Piperonyl butoxide

Other names:	1,3-Benzodioxole, 5-[[2-(2-butoxyethoxy)ethoxy]methyl]-6-propyl-
	Toluene, «alpha»-[2-(2-butoxyethoxy)ethoxy]-4,5-(methylenedioxy)-2-propyl-
	Butacide
	Butocide
	Butyl carbitol 6-propylpiperonyl ether
	ENT 14,250
	Pyrenone 606
	6-Propylpiperonyl butyl diethylene glycol ether
	«alpha»-(2-(2-n-Butoxyethoxy)-ethoxy)-4,5-methylenedioxy-2-propyltoluene
	«alpha»(2-(2-Butoxyethoxy)ethoxy)-4,5-methylenedioxy-2-propyltoluene
	(3,4-Methylenedioxy-6-propylbenzyl) (butyl) diethylene glycol ether
	Butylcarbityl (6-propylpiperonyl) ether
	Ethanol butoxide
	FMC 5273
	NCI-C02813
	NIA 5273
	PB
	3,4-Methylendioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether
	3,4-Methylenedioxy-6-propylbenzyl n-butyl diethyleneglycol ether
	5-Propyl-4-(2,5,8-trioxa-dodecyl)-1,3-benzodioxole
	6-(Propylpiperonyl)butylcarbityl ether
	Butoxide
	FAC 5273
	Nusyn-noxfish
	Pyrenon
	4,5-Methylenedioxy-2-propylbenzyldiethylene glycol butyl ether
	Alleviate
	Butoxide (synergist)
	PBO
	NSC 8401
	2-(2-butoxyethoxy)ethyl 6-propylpiperonyl ether
Inchi:	InChI=1S/C19H30O5/c1-3-5-7-20-8-9-21-10-11-22-14-17-13-19-18(23-15-24-19)12-16(1
InchiKey:	FIPWRIJSWJWJAI-UHFFFAOYSA-N
Formula:	C19H30O5
SMILES:	CCCCOCCOCCOCc1cc2c(cc1CCC)OCO2
Mol. weight [g/mol]:	338.44
CAS:	51-03-6

Physical Properties

Property code	Value	Unit	Source
gf	-226.16	kJ/mol	Joback Method
hf	-800.89	kJ/mol	Joback Method
hfus	54.43	kJ/mol	Joback Method
hvap	78.62	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.718		Crippen Method
mcvol	273.300	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	2407.00		NIST Webbook
rinpol	2358.00		NIST Webbook
rinpol	2366.00		NIST Webbook
rinpol	2366.00		NIST Webbook
rinpol	2407.00		NIST Webbook
ripol	3235.00		NIST Webbook
ripol	3235.00		NIST Webbook
tb	808.31	K	Joback Method
tc	1004.95	K	Joback Method
tf	509.88	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.65	J/mol×K	808.31	Joback Method
cpg	929.24	J/mol×K	972.18	Joback Method
cpg	916.26	J/mol×K	939.40	Joback Method
cpg	902.34	J/mol×K	906.63	Joback Method
cpg	887.45	J/mol×K	873.86	Joback Method
cpg	871.56	J/mol×K	841.08	Joback Method
cpg	941.29	J/mol×K	1004.95	Joback Method
dvisc	0.0000921	Pa×s	808.31	Joback Method
dvisc	0.0001131	Pa×s	758.57	Joback Method
dvisc	0.0001430	Pa×s	708.83	Joback Method
dvisc	0.0001872	Pa×s	659.10	Joback Method
dvisc	0.0002561	Pa×s	609.36	Joback Method
dvisc	0.0003704	Pa×s	559.62	Joback Method

dvisc	0.0005758	Pa×s	509.88	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.20	K	0.04	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51036&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume