Diethylene glycol dibenzoate

Other names:	2,2'-Oxydiethylene dibenzoate
	2-[2-(Benzoyloxy)ethoxy]ethyl benzoate
	Benzo Flex 2-45
	Benzoic acid, diester with diethylene glycol
	Dibenzoyldiethyleneglycol ester
	Diglycol dibenzoate
	Ethanol, 2,2'-oxybis-, 1,1'-dibenzoate
	Ethanol, 2,2'-oxybis-, dibenzoate
	oxybis(ethane-2,1-diyl) dibenzoate
	oxydiethylene dibenzoate
Inchi:	InChI=1S/C18H18O5/c19-17(15-7-3-1-4-8-15)22-13-11-21-12-14-23-18(20)16-9-5-2-6-10
InchiKey:	NXQMCAOPTPLPRL-UHFFFAOYSA-N
Formula:	C18H18O5
SMILES:	O=C(OCCOCCOC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	314.33
CAS:	120-55-8

Physical Properties

Property code	Value	Unit	Source
gf	-247.34	kJ/mol	Joback Method
hf	-563.61	kJ/mol	Joback Method
hfus	37.22	kJ/mol	Joback Method
hvap	80.94	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.717		Crippen Method
mcvol	237.710	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
tb	839.60	K	Joback Method
tc	1065.56	K	Joback Method
tf	512.01	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.70	J/mol×K	1065.56	Joback Method
cpg	750.54	J/mol×K	1027.90	Joback Method
cpg	742.17	J/mol×K	990.24	Joback Method
cpg	732.56	J/mol×K	952.58	Joback Method
cpg	721.70	J/mol×K	914.92	Joback Method
cpg	709.55	J/mol×K	877.26	Joback Method
cpg	696.11	J/mol×K	839.60	Joback Method
dvisc	0.0005119	Pa×s	512.01	Joback Method
dvisc	0.0000549	Pa×s	839.60	Joback Method
dvisc	0.0000699	Pa×s	785.00	Joback Method
dvisc	0.0000924	Pa×s	730.40	Joback Method
dvisc	0.0001278	Pa×s	675.80	Joback Method
dvisc	0.0001871	Pa×s	621.21	Joback Method
dvisc	0.0002949	Pa×s	566.61	Joback Method
pvap	1.02	kPa	511.35	Experimental Isobaric Vapor Liquid Equilibrium for Binary Systems Diethylene Glycol Dibenzoate + Diethylene Glycol, Diethylene Glycol Dibenzoate + Octyl Benzoate, and Ternary System Diethylene Glycol Dibenzoate + Diethylene Glycol + Octyl Benzoate at 1.0152 kPa

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental Isobaric Vapor Liquid Equilibrium for Binary Systems Diethylene Glycol Dibenzoate + Diethylene Glycol, Diethylene Glycol Dibenzoate + Octyl Benzoate, and Ternary System Diethylene Glycol Dibenzoate + Diethylene Glycol + Octyl Benzoate at 1.0152 kPa:	https://www.doi.org/10.1021/acs.jced.8b00460
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120558&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume