1,3-Dioxolane, 2-ethyl-4-((4-phenoxyphenoxy)methyl)-

Other names: 2-Ethyl-4-[(4-phenoxyphenoxy)methyl]-1,3-dioxolane
Diofenolan

Inchi: InChI=1S/C18H20O4/c1-2-18-20-13-17(22-18)12-19-14-8-10-16(11-9-14)21-15-6-4-3-5-7

InchiKey: ZDOOQPFIGYHZFV-UHFFFAOYSA-N

Formula: C18H20O4

SMILES: CCC1OCC(COc2ccc(Oc3ccccc3)cc2)O1

Mol. weight [g/mol]: 300.35

CAS: 63837-33-2

Physical Properties

Property code	Value	Unit	Source
gf	-37.53	kJ/mol	Joback Method
hf	-441.56	kJ/mol	Joback Method
hfus	43.41	kJ/mol	Joback Method
hvap	74.66	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	4.009		Crippen Method
mcvol	229.580	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	2459.00		NIST Webbook
rinpol	2459.00		NIST Webbook
tb	778.93	K	Joback Method
tc	1017.42	K	Joback Method
tf	462.24	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.22	J/mol×K	778.93	Joback Method
cpg	711.17	J/mol×K	818.68	Joback Method
cpg	727.56	J/mol×K	858.43	Joback Method
cpg	742.42	J/mol×K	898.17	Joback Method
cpg	755.81	J/mol×K	937.92	Joback Method

cpg	767.77	J/mol×K	977.67	Joback Method
cpg	778.33	J/mol×K	1017.42	Joback Method
dvisc	0.0008967	Pa×s	462.24	Joback Method
dvisc	0.0005288	Pa×s	515.02	Joback Method
dvisc	0.0003440	Pa×s	567.80	Joback Method
dvisc	0.0002408	Pa×s	620.59	Joback Method
dvisc	0.0001782	Pa×s	673.37	Joback Method
dvisc	0.0001378	Pa×s	726.15	Joback Method
dvisc	0.0001103	Pa×s	778.93	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C63837332&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume