2,4-dichlorobenzyl tetradecyl ether

Inchi: InChI=1S/C21H34Cl2O/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-24-18-19-14-15-20(22)17-21(
InchiKey: HAAXOBRRZGCQCL-UHFFFAOYSA-N
Formula: C21H34Cl2O
SMILES: CCCCCCCCCCCCCCCOCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 373.40

Physical Properties

Property code	Value	Unit	Source
gf	90.23	kJ/mol	Joback Method
hf	-426.88	kJ/mol	Joback Method
hfus	52.99	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	8.211		Crippen Method
mcvol	313.340	ml/mol	McGowan Method
pc	1093.54	kPa	Joback Method
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2594.00		NIST Webbook
rinpol	2595.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2589.00		NIST Webbook
rinpol	2594.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2588.00		NIST Webbook
rinpol	2588.00		NIST Webbook
tb	813.80	K	Joback Method
tc	1008.30	K	Joback Method
tf	459.96	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.53	J/mol×K	813.80	Joback Method
cpg	942.32	J/mol×K	846.22	Joback Method
cpg	959.07	J/mol×K	878.63	Joback Method
cpg	974.82	J/mol×K	911.05	Joback Method
cpg	989.60	J/mol×K	943.46	Joback Method
cpg	1003.45	J/mol×K	975.88	Joback Method
cpg	1016.41	J/mol×K	1008.30	Joback Method
dvisc	0.0006528	Pa×s	459.96	Joback Method
dvisc	0.0003364	Pa×s	518.93	Joback Method
dvisc	0.0001985	Pa×s	577.91	Joback Method
dvisc	0.0001291	Pa×s	636.88	Joback Method
dvisc	0.0000903	Pa×s	695.85	Joback Method
dvisc	0.0000668	Pa×s	754.83	Joback Method
dvisc	0.0000517	Pa×s	813.80	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R32361&Units=SI

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