2,4-dichlorobenzyl hexadecyl ether

Inchi: InChI=1S/C23H38Cl2O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-26-20-21-16-17-22(24)
InchiKey: IVKTUGKMWWUJHF-UHFFFAOYSA-N
Formula: C23H38Cl2O
SMILES: CCCCCCCCCCCCCCCCOCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 401.45

Physical Properties

Property code	Value	Unit	Source
gf	107.07	kJ/mol	Joback Method
hf	-468.16	kJ/mol	Joback Method
hfus	58.17	kJ/mol	Joback Method
hvap	81.57	kJ/mol	Joback Method
log10ws	-9.51		Crippen Method
logp	8.991		Crippen Method
mcvol	341.520	ml/mol	McGowan Method
pc	966.87	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2808.00		NIST Webbook
rinpol	2813.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2804.00		NIST Webbook
rinpol	2808.00		NIST Webbook
rinpol	2804.00		NIST Webbook
rinpol	2812.00		NIST Webbook
rinpol	2806.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2813.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2810.00		NIST Webbook
tb	859.56	K	Joback Method
tc	1057.11	K	Joback Method
tf	482.50	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1045.56	J/mol×K	859.56	Joback Method
cpg	1063.93	J/mol×K	892.49	Joback Method
cpg	1081.18	J/mol×K	925.41	Joback Method
cpg	1097.36	J/mol×K	958.34	Joback Method
cpg	1112.50	J/mol×K	991.26	Joback Method
cpg	1126.66	J/mol×K	1024.19	Joback Method
cpg	1139.88	J/mol×K	1057.11	Joback Method
dvisc	0.0005303	Pa×s	482.50	Joback Method
dvisc	0.0002671	Pa×s	545.34	Joback Method
dvisc	0.0001550	Pa×s	608.19	Joback Method
dvisc	0.0000996	Pa×s	671.03	Joback Method
dvisc	0.0000690	Pa×s	733.87	Joback Method
dvisc	0.0000507	Pa×s	796.72	Joback Method
dvisc	0.0000390	Pa×s	859.56	Joback Method

Sources

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=R32290&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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