

2,4-dichlorobenzyl tridecyl ether

Inchi: InChI=1S/C20H32Cl2O/c1-2-3-4-5-6-7-8-9-10-11-12-15-23-17-18-13-14-19(21)16-20(18)
InchiKey: OTSXSHIAJZTAFV-UHFFFAOYSA-N
Formula: C20H32Cl2O
SMILES: CCCCCCCCCCCCCOCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 359.37

Physical Properties

Property code	Value	Unit	Source
gf	81.81	kJ/mol	Joback Method
hf	-406.24	kJ/mol	Joback Method
hfus	50.40	kJ/mol	Joback Method
hvap	74.89	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	7.821		Crippen Method
mcvol	299.250	ml/mol	McGowan Method
pc	1166.43	kPa	Joback Method
rinpol	2495.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2483.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2496.00		NIST Webbook
rinpol	2483.00		NIST Webbook
rinpol	2491.00		NIST Webbook
rinpol	2494.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2483.00		NIST Webbook
tb	790.92	K	Joback Method
tc	984.93	K	Joback Method
tf	448.69	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.24	J/molxK	790.92	Joback Method
cpg	882.75	J/molxK	823.25	Joback Method
cpg	899.26	J/molxK	855.59	Joback Method
cpg	914.80	J/molxK	887.92	Joback Method
cpg	929.40	J/molxK	920.26	Joback Method
cpg	943.08	J/molxK	952.59	Joback Method
cpg	955.90	J/molxK	984.93	Joback Method
dvisc	0.0007196	Paxs	448.69	Joback Method
dvisc	0.0003753	Paxs	505.73	Joback Method
dvisc	0.0002234	Paxs	562.77	Joback Method
dvisc	0.0001463	Paxs	619.80	Joback Method
dvisc	0.0001029	Paxs	676.84	Joback Method
dvisc	0.0000764	Paxs	733.88	Joback Method
dvisc	0.0000592	Paxs	790.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R32375&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

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