

Sebacic acid, 2,3-dichlorophenyl isobutyl ester

Inchi:	InChI=1S/C20H28Cl2O4/c1-15(2)14-25-18(23)12-7-5-3-4-6-8-13-19(24)26-17-11-9-10-16
InchiKey:	HGTFVSWLZGKKPM-UHFFFAOYSA-N
Formula:	C20H28Cl2O4
SMILES:	CC(C)COC(=O)CCCCCCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	403.34

Physical Properties

Property code	Value	Unit	Source
gf	-283.47	kJ/mol	Joback Method
hf	-768.90	kJ/mol	Joback Method
hfus	51.26	kJ/mol	Joback Method
hvap	90.41	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.219		Crippen Method
mcvol	308.260	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinqol	2866.00		NIST Webbook
tb	920.64	K	Joback Method
tc	1133.87	K	Joback Method
tf	555.78	K	Joback Method
vc	1.188	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.62	J/molxK	920.64	Joback Method
cpg	986.48	J/molxK	1098.33	Joback Method
cpg	977.44	J/molxK	1062.79	Joback Method
cpg	967.26	J/molxK	1027.25	Joback Method
cpg	955.91	J/molxK	991.72	Joback Method
cpg	943.37	J/molxK	956.18	Joback Method
cpg	994.41	J/molxK	1133.87	Joback Method
dvisc	0.0000374	Paxs	920.64	Joback Method
dvisc	0.0000480	Paxs	859.83	Joback Method

dvisc	0.0000640	Paxs	799.02	Joback Method
dvisc	0.0000893	Paxs	738.21	Joback Method
dvisc	0.0001325	Paxs	677.40	Joback Method
dvisc	0.0002124	Paxs	616.59	Joback Method
dvisc	0.0003776	Paxs	555.78	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=U354941&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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