

Sebacic acid, 2,3-dichlorobenzyl isobutyl ester

Inchi:	InChI=1S/C21H30Cl2O4/c1-16(2)14-26-19(24)12-7-5-3-4-6-8-13-20(25)27-15-17-10-9-1
InchiKey:	JLGVSZYEVPYRIK-UHFFFAOYSA-N
Formula:	C21H30Cl2O4
SMILES:	CC(C)COC(=O)CCCCCCCCC(=O)OCc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	417.37

Physical Properties

Property code	Value	Unit	Source
gf	-275.05	kJ/mol	Joback Method
hf	-789.54	kJ/mol	Joback Method
hfus	53.85	kJ/mol	Joback Method
hvap	92.63	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.357		Crippen Method
mcvol	322.350	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2921.00		NIST Webbook
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tb	943.52	K	Joback Method
tc	1158.79	K	Joback Method
tf	567.05	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.90	J/molxK	943.52	Joback Method
cpg	1002.83	J/molxK	979.40	Joback Method
cpg	1015.48	J/molxK	1015.28	Joback Method
cpg	1026.90	J/molxK	1051.16	Joback Method
cpg	1037.09	J/molxK	1087.04	Joback Method
cpg	1046.10	J/molxK	1122.92	Joback Method
cpg	1053.96	J/molxK	1158.79	Joback Method
dvisc	0.0003367	Paxs	567.05	Joback Method

dvisc	0.0001874	Paxs	629.79	Joback Method
dvisc	0.0001159	Paxs	692.54	Joback Method
dvisc	0.0000777	Paxs	755.28	Joback Method
dvisc	0.0000554	Paxs	818.03	Joback Method
dvisc	0.0000414	Paxs	880.77	Joback Method
dvisc	0.0000322	Paxs	943.52	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=U380601&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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