Sebacic acid, 2,5-dichlorobenzyl isobutyl ester

Inchi: InChI=1S/C21H30Cl2O4/c1-16(2)14-26-20(24)9-7-5-3-4-6-8-10-21(25)27-15-17-13-18(22
InchiKey: IGMLFKOUSKPDED-UHFFFAOYSA-N
Formula: C21H30Cl2O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1cc(Cl)ccc1Cl
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	2872.00		NIST Webbook
rinpol	2872.00		NIST Webbook
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/mol×K	943.52	Joback Method
cpg	1046.10	J/mol×K	1122.92	Joback Method
cpg	1037.09	J/mol×K	1087.04	Joback Method
cpg	1026.90	J/mol×K	1051.16	Joback Method
cpg	1015.48	J/mol×K	1015.28	Joback Method
cpg	1002.83	J/mol×K	979.40	Joback Method
cpg	1053.96	J/mol×K	1158.79	Joback Method
dvisc	0.0000322	Pa×s	943.52	Joback Method

dvisc	0.0000414	Pa×s	880.77	Joback Method
dvisc	0.0000554	Pa×s	818.03	Joback Method
dvisc	0.0000777	Pa×s	755.28	Joback Method
dvisc	0.0001159	Pa×s	692.54	Joback Method
dvisc	0.0001874	Pa×s	629.79	Joback Method
dvisc	0.0003367	Pa×s	567.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380612&Units=SI
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

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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