Sebacic acid, 2,4-dichlorophenethyl propyl ester

Inchi: InChI=1S/C21H30Cl2O4/c1-2-14-26-20(24)9-7-5-3-4-6-8-10-21(25)27-15-13-17-11-12-18

InchiKey: KZXGPOHPWCSWIS-UHFFFAOYSA-N

Formula: C21H30Cl2O4

SMILES: CCCOC(=O)CCCCCCCCC(=O)OCCc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 417.37

Physical Properties

Property code	Value	Unit	Source
gf	-272.61	kJ/mol	Joback Method
hf	-784.26	kJ/mol	Joback Method
hfus	57.38	kJ/mol	Joback Method
hvap	93.02	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	6.153		Crippen Method
mcvol	322.350	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	2822.00		NIST Webbook
rinpol	2822.00		NIST Webbook
tb	943.96	K	Joback Method
tc	1158.36	K	Joback Method
tf	582.05	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.45	J/mol×K	943.96	Joback Method
cpg	1045.81	J/mol×K	1122.62	Joback Method
cpg	1036.72	J/mol×K	1086.89	Joback Method
cpg	1026.47	J/mol×K	1051.16	Joback Method
cpg	1015.03	J/mol×K	1015.43	Joback Method
cpg	1002.36	J/mol×K	979.69	Joback Method
cpg	1053.76	J/mol×K	1158.36	Joback Method
dvisc	0.0000353	Pa×s	943.96	Joback Method

dvisc	0.0000448	Pa×s	883.64	Joback Method
dvisc	0.0000589	Pa×s	823.32	Joback Method
dvisc	0.0000809	Pa×s	763.00	Joback Method
dvisc	0.0001172	Pa×s	702.69	Joback Method
dvisc	0.0001821	Pa×s	642.37	Joback Method
dvisc	0.0003100	Pa×s	582.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416816&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

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