Sebacic acid, di(2,2-dichloroethyl) ester

Inchi: InChI=1S/C14H22Cl4O4/c15-11(16)9-21-13(19)7-5-3-1-2-4-6-8-14(20)22-10-12(17)18/h1
InchiKey: UUYXFUXOPDQHKU-UHFFFAOYSA-N
Formula: C14H22Cl4O4
SMILES: O=C(CCCCCCCCC(=O)OCC(Cl)Cl)OCC(Cl)Cl
Mol. weight [g/mol]: 396.13

Physical Properties

Property code	Value	Unit	Source
gf	-453.44	kJ/mol	Joback Method
hf	-895.41	kJ/mol	Joback Method
hfus	47.33	kJ/mol	Joback Method
hvap	81.83	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.801		Crippen Method
mcvol	271.960	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
tb	821.14	K	Joback Method
tc	1020.17	K	Joback Method
tf	481.54	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.38	J/mol×K	821.14	Joback Method
cpg	787.54	J/mol×K	987.00	Joback Method
cpg	778.64	J/mol×K	953.83	Joback Method
cpg	768.89	J/mol×K	920.66	Joback Method
cpg	758.27	J/mol×K	887.48	Joback Method
cpg	746.77	J/mol×K	854.31	Joback Method
cpg	795.60	J/mol×K	1020.17	Joback Method
dvisc	0.0000579	Pa×s	821.14	Joback Method

dvisc	0.0000767	Pa×s	764.54	Joback Method
dvisc	0.0001064	Pa×s	707.94	Joback Method
dvisc	0.0001562	Pa×s	651.34	Joback Method
dvisc	0.0002466	Pa×s	594.74	Joback Method
dvisc	0.0004286	Pa×s	538.14	Joback Method
dvisc	0.0008483	Pa×s	481.54	Joback Method

Sources

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=U355479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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