Sebacic acid, 2,2-dichloroethyl tetradecyl ester

Inchi: InChI=1S/C26H48Cl2O4/c1-2-3-4-5-6-7-8-9-10-13-16-19-22-31-25(29)20-17-14-11-12-15

InchiKey: DHGHTMNOYLPULJ-UHFFFAOYSA-N

Formula: C26H48Cl2O4

SMILES: CCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 495.56

Physical Properties

Property code	Value	Unit	Source
gf	-326.10	kJ/mol	Joback Method
hf	-1106.33	kJ/mol	Joback Method
hfus	73.54	kJ/mol	Joback Method
hvap	100.16	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.698		Crippen Method
mcvol	416.560	ml/mol	McGowan Method
pc	735.22	kPa	Joback Method
rinpol	3348.00		NIST Webbook
rinpol	3348.00		NIST Webbook
tb	1021.28	K	Joback Method
tc	1264.12	K	Joback Method
tf	571.94	K	Joback Method
vc	1.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1403.70	J/mol×K	1021.28	Joback Method
cpg	1481.67	J/mol×K	1223.65	Joback Method
cpg	1469.55	J/mol×K	1183.18	Joback Method
cpg	1455.77	J/mol×K	1142.70	Joback Method
cpg	1440.25	J/mol×K	1102.23	Joback Method
cpg	1422.92	J/mol×K	1061.75	Joback Method
cpg	1492.20	J/mol×K	1264.12	Joback Method
dvisc	0.0000135	Pa×s	1021.28	Joback Method

dvisc	0.0000183	Pa×s	946.39	Joback Method
dvisc	0.0000260	Pa×s	871.50	Joback Method
dvisc	0.0000394	Pa×s	796.61	Joback Method
dvisc	0.0000653	Pa×s	721.72	Joback Method
dvisc	0.0001216	Pa×s	646.83	Joback Method
dvisc	0.0002665	Pa×s	571.94	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=U355477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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