Sebacic acid, 2,2-dichloroethyl pentadecyl ester

Inchi: InChI=1S/C27H50Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-20-23-32-26(30)21-18-15-12-13

InchiKey: VAKDUWZYDMTKEF-UHFFFAOYSA-N

Formula: C27H50Cl2O4

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

Mol. weight [g/mol]: 509.59

Physical Properties

Property code	Value	Unit	Source
gf	-317.68	kJ/mol	Joback Method
hf	-1126.97	kJ/mol	Joback Method
hfus	76.13	kJ/mol	Joback Method
hvap	102.39	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	9.088		Crippen Method
mcvol	430.650	ml/mol	McGowan Method
pc	698.39	kPa	Joback Method
rinpol	3458.00		NIST Webbook
tb	1044.16	K	Joback Method
tc	1298.76	K	Joback Method
tf	583.21	K	Joback Method
vc	1.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1467.32	J/mol×K	1044.16	Joback Method
cpg	1487.13	J/mol×K	1086.59	Joback Method
cpg	1504.86	J/mol×K	1129.03	Joback Method
cpg	1520.59	J/mol×K	1171.46	Joback Method
cpg	1534.43	J/mol×K	1213.89	Joback Method
cpg	1546.46	J/mol×K	1256.32	Joback Method
cpg	1556.78	J/mol×K	1298.76	Joback Method
dvisc	0.0002316	Pa×s	583.21	Joback Method
dvisc	0.0001049	Pa×s	660.03	Joback Method

dvisc	0.0000560	Pa×s	736.86	Joback Method
dvisc	0.0000337	Pa×s	813.68	Joback Method
dvisc	0.0000221	Pa×s	890.51	Joback Method
dvisc	0.0000155	Pa×s	967.33	Joback Method
dvisc	0.0000115	Pa×s	1044.16	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=U355478&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