Adipic acid, 2,2-dichloroethyl heptadecyl ester

Inchi: InChI=1S/C25H46Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-30-24(28)19-16-17
InchiKey: FYKQPNLKSKQJRZ-UHFFFAOYSA-N
Formula: C25H46Cl2O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 481.54

Physical Properties

Property code	Value	Unit	Source
gf	-334.52	kJ/mol	Joback Method
hf	-1085.69	kJ/mol	Joback Method
hfus	70.95	kJ/mol	Joback Method
hvap	97.94	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	8.308		Crippen Method
mcvol	402.470	ml/mol	McGowan Method
pc	775.05	kPa	Joback Method
rinpol	3206.00		NIST Webbook
rinpol	3206.00		NIST Webbook
tb	998.40	K	Joback Method
tc	1230.91	K	Joback Method
tf	560.67	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1340.42	J/mol×K	998.40	Joback Method
cpg	1359.09	J/mol×K	1037.15	Joback Method
cpg	1376.04	J/mol×K	1075.90	Joback Method
cpg	1391.33	J/mol×K	1114.66	Joback Method
cpg	1405.03	J/mol×K	1153.41	Joback Method
cpg	1417.19	J/mol×K	1192.16	Joback Method
cpg	1427.88	J/mol×K	1230.91	Joback Method
dvisc	0.0003061	Pa×s	560.67	Joback Method

dvisc	0.0001408	Pa×s	633.62	Joback Method
dvisc	0.0000760	Pa×s	706.58	Joback Method
dvisc	0.0000461	Pa×s	779.53	Joback Method
dvisc	0.0000304	Pa×s	852.49	Joback Method
dvisc	0.0000214	Pa×s	925.44	Joback Method
dvisc	0.0000159	Pa×s	998.40	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=U353591&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