

Adipic acid, 2,2-dichloroethyl tetradecyl ester

Inchi: InChI=1S/C22H40Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-27-21(25)16-13-14-17-22(26)23-24
InchiKey: UGOXCFYVYCYWDZ-UHFFFAOYSA-N
Formula: C22H40Cl2O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 439.46

Physical Properties

Property code	Value	Unit	Source
gf	-359.78	kJ/mol	Joback Method
hf	-1023.77	kJ/mol	Joback Method
hfus	63.18	kJ/mol	Joback Method
hvap	91.26	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	7.138		Crippen Method
mvol	360.200	ml/mol	McGowan Method
pc	916.05	kPa	Joback Method
rinpol	2898.00		NIST Webbook
rinpol	2898.00		NIST Webbook
tb	929.76	K	Joback Method
tc	1138.78	K	Joback Method
tf	526.86	K	Joback Method
vc	1.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.06	J/molxK	929.76	Joback Method
cpg	1170.30	J/molxK	964.60	Joback Method
cpg	1186.20	J/molxK	999.43	Joback Method
cpg	1200.80	J/molxK	1034.27	Joback Method
cpg	1214.13	J/molxK	1069.11	Joback Method
cpg	1226.23	J/molxK	1103.94	Joback Method
cpg	1237.14	J/molxK	1138.78	Joback Method
dvisc	0.0004577	Paxs	526.86	Joback Method

dvisc	0.0002160	Paxs	594.01	Joback Method
dvisc	0.0001188	Paxs	661.16	Joback Method
dvisc	0.0000729	Paxs	728.31	Joback Method
dvisc	0.0000486	Paxs	795.46	Joback Method
dvisc	0.0000345	Paxs	862.61	Joback Method
dvisc	0.0000257	Paxs	929.76	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=U353588&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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