

Adipic acid, 2,2-dichloroethyl hexadecyl ester

Inchi:	InChI=1S/C24H44Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-29-23(27)18-15-16-19
InchiKey:	QYCHWEMELRPFJS-UHFFFAOYSA-N
Formula:	C24H44Cl2O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	467.51

Physical Properties

Property code	Value	Unit	Source
gf	-342.94	kJ/mol	Joback Method
hf	-1065.05	kJ/mol	Joback Method
hfus	68.36	kJ/mol	Joback Method
hvap	95.71	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.918		Crippen Method
mvol	388.380	ml/mol	McGowan Method
pc	818.20	kPa	Joback Method
rinpol	3104.00		NIST Webbook
tb	975.52	K	Joback Method
tc	1199.01	K	Joback Method
tf	549.40	K	Joback Method
vc	1.520	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.51	J/molxK	975.52	Joback Method
cpg	1295.68	J/molxK	1012.77	Joback Method
cpg	1312.26	J/molxK	1050.02	Joback Method
cpg	1327.33	J/molxK	1087.27	Joback Method
cpg	1340.92	J/molxK	1124.52	Joback Method
cpg	1353.08	J/molxK	1161.76	Joback Method
cpg	1363.88	J/molxK	1199.01	Joback Method
dvisc	0.0003509	Paxs	549.40	Joback Method
dvisc	0.0001627	Paxs	620.42	Joback Method

dvisc	0.0000884	Paxs	691.44	Joback Method
dvisc	0.0000538	Paxs	762.46	Joback Method
dvisc	0.0000356	Paxs	833.48	Joback Method
dvisc	0.0000252	Paxs	904.50	Joback Method
dvisc	0.0000187	Paxs	975.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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