Adipic acid, 2,2-dichloroethyl propyl ester

Inchi: InChI=1S/C11H18Cl2O4/c1-2-7-16-10(14)5-3-4-6-11(15)17-8-9(12)13/h9H,2-8H2,1H3
InchiKey: SAFVILILGJGGST-UHFFFAOYSA-N
Formula: C11H18Cl2O4
SMILES: CCCOC(=O)CCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 285.16

Physical Properties

Property code	Value	Unit	Source
gf	-452.40	kJ/mol	Joback Method
hf	-796.73	kJ/mol	Joback Method
hfus	34.69	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.847		Crippen Method
mcvol	205.210	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	678.08	K	Joback Method
tc	868.17	K	Joback Method
tf	402.89	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.24	J/mol×K	678.08	Joback Method
cpg	578.00	J/mol×K	836.49	Joback Method
cpg	568.00	J/mol×K	804.80	Joback Method
cpg	557.33	J/mol×K	773.12	Joback Method
cpg	545.98	J/mol×K	741.44	Joback Method
cpg	533.95	J/mol×K	709.76	Joback Method
cpg	587.33	J/mol×K	868.17	Joback Method
dvisc	0.0001309	Pa×s	678.08	Joback Method

dvisc	0.0001703	Pa×s	632.21	Joback Method
dvisc	0.0002310	Pa×s	586.35	Joback Method
dvisc	0.0003300	Pa×s	540.48	Joback Method
dvisc	0.0005035	Pa×s	494.62	Joback Method
dvisc	0.0008376	Pa×s	448.75	Joback Method
dvisc	0.0015647	Pa×s	402.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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