

Adipic acid, 2,2-dichloroethyl isoheptyl ester

Inchi: InChI=1S/C14H24Cl2O4/c1-11(2)6-5-9-19-13(17)7-3-4-8-14(18)20-10-12(15)16/h11-12H
InchiKey: PFPKASMI BHPKPN-UHFFFAOYSA-N
Formula: C14H24Cl2O4
SMILES: CC(C)CCCOC(=O)CCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 327.24

Physical Properties

Property code	Value	Unit	Source
gf	-429.58	kJ/mol	Joback Method
hf	-863.93	kJ/mol	Joback Method
hfus	38.94	kJ/mol	Joback Method
hvap	73.06	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.873		Crippen Method
mvol	247.480	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	2110.00		NIST Webbook
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tb	746.28	K	Joback Method
tc	936.02	K	Joback Method
tf	421.70	K	Joback Method
vc	0.954	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.41	J/molxK	746.28	Joback Method
cpg	696.76	J/molxK	777.90	Joback Method
cpg	710.26	J/molxK	809.53	Joback Method
cpg	722.93	J/molxK	841.15	Joback Method
cpg	734.78	J/molxK	872.77	Joback Method
cpg	745.80	J/molxK	904.40	Joback Method
cpg	756.02	J/molxK	936.02	Joback Method
dvisc	0.0014066	Paxs	421.70	Joback Method

dvisc	0.0006641	Paxs	475.80	Joback Method
dvisc	0.0003655	Paxs	529.89	Joback Method
dvisc	0.0002247	Paxs	583.99	Joback Method
dvisc	0.0001500	Paxs	638.09	Joback Method
dvisc	0.0001067	Paxs	692.18	Joback Method
dvisc	0.0000797	Paxs	746.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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