

Adipic acid, isohexyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C14H23Cl3O4/c1-11(2)6-5-9-20-12(18)7-3-4-8-13(19)21-10-14(15,16)17/h11H
InchiKey:	OGDSRLIYUZDTOX-UHFFFAOYSA-N
Formula:	C14H23Cl3O4
SMILES:	CC(C)CCCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	361.69

Physical Properties

Property code	Value	Unit	Source
gf	-436.23	kJ/mol	Joback Method
hf	-883.14	kJ/mol	Joback Method
hfus	39.24	kJ/mol	Joback Method
hvap	76.54	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.440		Crippen Method
mcvol	259.720	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinsol	2122.00		NIST Webbook
tb	780.92	K	Joback Method
tc	979.19	K	Joback Method
tf	469.04	K	Joback Method
vc	0.998	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.63	J/molxK	780.92	Joback Method
cpg	768.85	J/molxK	946.15	Joback Method
cpg	758.88	J/molxK	913.10	Joback Method
cpg	748.09	J/molxK	880.06	Joback Method
cpg	736.48	J/molxK	847.01	Joback Method
cpg	724.00	J/molxK	813.97	Joback Method
cpg	778.05	J/molxK	979.19	Joback Method
dvisc	0.0000602	Paxs	780.92	Joback Method
dvisc	0.0000803	Paxs	728.94	Joback Method

dvisc	0.0001120	Paxs	676.96	Joback Method
dvisc	0.0001651	Paxs	624.98	Joback Method
dvisc	0.0002611	Paxs	573.00	Joback Method
dvisc	0.0004524	Paxs	521.02	Joback Method
dvisc	0.0008856	Paxs	469.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353478&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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