

Adipic acid, pentyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C13H21Cl3O4/c1-2-3-6-9-19-11(17)7-4-5-8-12(18)20-10-13(14,15)16/h2-10H2
InchiKey:	IOYNASRZSJQINR-UHFFFAOYSA-N
Formula:	C13H21Cl3O4
SMILES:	CCCCCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	347.66

Physical Properties

Property code	Value	Unit	Source
gf	-442.21	kJ/mol	Joback Method
hf	-857.22	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	74.70	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.194		Crippen Method
mvol	245.630	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2063.00		NIST Webbook
rinpol	2063.00		NIST Webbook
tb	758.48	K	Joback Method
tc	955.08	K	Joback Method
tf	472.77	K	Joback Method
vc	0.948	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.24	J/molxK	758.48	Joback Method
cpg	668.06	J/molxK	791.25	Joback Method
cpg	680.05	J/molxK	824.01	Joback Method
cpg	691.24	J/molxK	856.78	Joback Method
cpg	701.65	J/molxK	889.54	Joback Method
cpg	711.30	J/molxK	922.31	Joback Method
cpg	720.23	J/molxK	955.08	Joback Method
dvisc	0.0008519	Paxs	472.77	Joback Method

dvisc	0.0004743	Paxs	520.39	Joback Method
dvisc	0.0002913	Paxs	568.01	Joback Method
dvisc	0.0001929	Paxs	615.62	Joback Method
dvisc	0.0001356	Paxs	663.24	Joback Method
dvisc	0.0000999	Paxs	710.86	Joback Method
dvisc	0.0000765	Paxs	758.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

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