

Adipic acid, decyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C18H31Cl3O4/c1-2-3-4-5-6-7-8-11-14-24-16(22)12-9-10-13-17(23)25-15-18(19)
InchiKey: CSQNQEAYEJCACP-UHFFFAOYSA-N
Formula: C18H31Cl3O4
SMILES: CCCCCCCCCCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 417.80

Physical Properties

Property code	Value	Unit	Source
gf	-400.11	kJ/mol	Joback Method
hf	-960.42	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	85.83	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.144		Crippen Method
mvol	316.080	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	2566.00		NIST Webbook
rinpol	2566.00		NIST Webbook
tb	872.88	K	Joback Method
tc	1072.77	K	Joback Method
tf	529.12	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.85	J/molxK	872.88	Joback Method
cpg	953.46	J/molxK	906.19	Joback Method
cpg	967.05	J/molxK	939.51	Joback Method
cpg	979.68	J/molxK	972.82	Joback Method
cpg	991.37	J/molxK	1006.14	Joback Method
cpg	1002.17	J/molxK	1039.45	Joback Method
cpg	1012.11	J/molxK	1072.77	Joback Method
dvisc	0.0004661	Paxs	529.12	Joback Method

dvisc	0.0002444	Paxs	586.41	Joback Method
dvisc	0.0001438	Paxs	643.71	Joback Method
dvisc	0.0000922	Paxs	701.00	Joback Method
dvisc	0.0000633	Paxs	758.29	Joback Method
dvisc	0.0000458	Paxs	815.59	Joback Method
dvisc	0.0000345	Paxs	872.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353482&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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