

Adipic acid, decyl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C18H32Cl2O4/c1-2-3-4-5-6-7-8-11-14-23-17(21)12-9-10-13-18(22)24-15-16(19)
InchiKey:	ZWNHQBBRCGMXBX-UHFFFAOYSA-N
Formula:	C18H32Cl2O4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	383.35

Physical Properties

Property code	Value	Unit	Source
gf	-393.46	kJ/mol	Joback Method
hf	-941.21	kJ/mol	Joback Method
hfus	52.82	kJ/mol	Joback Method
hvap	82.36	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.578		Crippen Method
mvol	303.840	ml/mol	McGowan Method
pc	1172.83	kPa	Joback Method
rinpol	2496.00		NIST Webbook
rinpol	2496.00		NIST Webbook
tb	838.24	K	Joback Method
tc	1030.31	K	Joback Method
tf	481.78	K	Joback Method
vc	1.183	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.10	J/mol×K	838.24	Joback Method
cpg	926.78	J/mol×K	870.25	Joback Method
cpg	941.44	J/mol×K	902.26	Joback Method
cpg	955.10	J/mol×K	934.28	Joback Method
cpg	967.78	J/mol×K	966.29	Joback Method
cpg	979.49	J/mol×K	998.30	Joback Method
cpg	990.25	J/mol×K	1030.31	Joback Method
dvisc	0.0007539	Paxs	481.78	Joback Method

dvisc	0.0003701	Paxs	541.19	Joback Method
dvisc	0.0002092	Paxs	600.60	Joback Method
dvisc	0.0001310	Paxs	660.01	Joback Method
dvisc	0.0000886	Paxs	719.42	Joback Method
dvisc	0.0000637	Paxs	778.83	Joback Method
dvisc	0.0000479	Paxs	838.24	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353584&Units=SI

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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