

Adipic acid, 2,2-dichloroethyl octadecyl ester

Inchi:	InChI=1S/C26H48Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-31-25(29)20-17
InchiKey:	ZLAMHMGBKQCSAC-UHFFFAOYSA-N
Formula:	C26H48Cl2O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	495.56

Physical Properties

Property code	Value	Unit	Source
gf	-326.10	kJ/mol	Joback Method
hf	-1106.33	kJ/mol	Joback Method
hfus	73.54	kJ/mol	Joback Method
hvap	100.16	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.698		Crippen Method
mvol	416.560	ml/mol	McGowan Method
pc	735.22	kPa	Joback Method
rinpol	3309.00		NIST Webbook
rinpol	3309.00		NIST Webbook
tb	1021.28	K	Joback Method
tc	1264.12	K	Joback Method
tf	571.94	K	Joback Method
vc	1.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1403.70	J/molxK	1021.28	Joback Method
cpg	1422.92	J/molxK	1061.75	Joback Method
cpg	1440.25	J/molxK	1102.23	Joback Method
cpg	1455.77	J/molxK	1142.70	Joback Method
cpg	1469.55	J/molxK	1183.18	Joback Method
cpg	1481.67	J/molxK	1223.65	Joback Method
cpg	1492.20	J/molxK	1264.12	Joback Method
dvisc	0.0002665	Paxs	571.94	Joback Method

dvisc	0.0001216	Paxs	646.83	Joback Method
dvisc	0.0000653	Paxs	721.72	Joback Method
dvisc	0.0000394	Paxs	796.61	Joback Method
dvisc	0.0000260	Paxs	871.50	Joback Method
dvisc	0.0000183	Paxs	946.39	Joback Method
dvisc	0.0000135	Paxs	1021.28	Joback Method

Sources

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=U353592&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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