

Adipic acid, 2,2-dichloroethyl ethyl ester

Inchi:	InChI=1S/C10H16Cl2O4/c1-2-15-9(13)5-3-4-6-10(14)16-7-8(11)12/h8H,2-7H2,1H3
InchiKey:	OOGYTZLFFXWBIU-UHFFFAOYSA-N
Formula:	C10H16Cl2O4
SMILES:	CCOC(=O)CCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	271.14

Physical Properties

Property code	Value	Unit	Source
gf	-460.82	kJ/mol	Joback Method
hf	-776.09	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Joback Method
hvap	64.55	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.457		Crippen Method
mcvol	191.120	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1704.00		NIST Webbook
tb	655.20	K	Joback Method
tc	847.01	K	Joback Method
tf	391.62	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.31	J/mol×K	655.20	Joback Method
cpg	482.41	J/mol×K	687.17	Joback Method
cpg	493.88	J/mol×K	719.14	Joback Method
cpg	504.72	J/mol×K	751.11	Joback Method
cpg	514.92	J/mol×K	783.08	Joback Method
cpg	524.48	J/mol×K	815.04	Joback Method
cpg	533.42	J/mol×K	847.01	Joback Method
dvisc	0.0017020	Pa×s	391.62	Joback Method
dvisc	0.0009246	Pa×s	435.55	Joback Method

dvisc	0.0005617	Pa×s	479.48	Joback Method
dvisc	0.0003711	Pa×s	523.41	Joback Method
dvisc	0.0002614	Pa×s	567.34	Joback Method
dvisc	0.0001936	Pa×s	611.27	Joback Method
dvisc	0.0001493	Pa×s	655.20	Joback Method

Sources

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=U353575&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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