

Adipic acid, ethyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C10H15Cl3O4/c1-2-16-8(14)5-3-4-6-9(15)17-7-10(11,12)13/h2-7H2,1H3
InchiKey:	NEAFJDMKYTVQND-UHFFFAOYSA-N
Formula:	C10H15Cl3O4
SMILES:	CCOC(=O)CCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	305.58

Physical Properties

Property code	Value	Unit	Source
gf	-467.47	kJ/mol	Joback Method
hf	-795.30	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	68.02	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.023		Crippen Method
mcvol	203.360	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinsol	1769.00		NIST Webbook
tb	689.84	K	Joback Method
tc	891.41	K	Joback Method
tf	438.96	K	Joback Method
vc	0.779	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.68	J/molxK	689.84	Joback Method
cpg	547.38	J/molxK	857.82	Joback Method
cpg	538.82	J/molxK	824.22	Joback Method
cpg	529.59	J/molxK	790.63	Joback Method
cpg	519.67	J/molxK	757.03	Joback Method
cpg	509.04	J/molxK	723.44	Joback Method
cpg	555.28	J/molxK	891.41	Joback Method
dvisc	0.0001206	Paxs	689.84	Joback Method
dvisc	0.0001558	Paxs	648.03	Joback Method

dvisc	0.0002087	Paxs	606.21	Joback Method
dvisc	0.0002918	Paxs	564.40	Joback Method
dvisc	0.0004304	Paxs	522.59	Joback Method
dvisc	0.0006795	Paxs	480.77	Joback Method
dvisc	0.0011701	Paxs	438.96	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=U353473&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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