

Adipic acid, 2-chloropropyl isobutyl ester

Inchi:	InChI=1S/C13H23ClO4/c1-10(2)8-17-12(15)6-4-5-7-13(16)18-9-11(3)14/h10-11H,4-9H2,
InchiKey:	AORGGPWPLAEDGG-UHFFFAOYSA-N
Formula:	C13H23ClO4
SMILES:	CC(C)COC(=O)CCCC(=O)OCC(C)Cl
Mol. weight [g/mol]:	278.77

Physical Properties

Property code	Value	Unit	Source
gf	-426.07	kJ/mol	Joback Method
hf	-827.55	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	66.45	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.916		Crippen Method
mcvol	221.150	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinsol	1806.00		NIST Webbook
tb	685.97	K	Joback Method
tc	872.11	K	Joback Method
tf	380.51	K	Joback Method
vc	0.849	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.34	J/molxK	685.97	Joback Method
cpg	614.16	J/molxK	716.99	Joback Method
cpg	628.21	J/molxK	748.02	Joback Method
cpg	641.50	J/molxK	779.04	Joback Method
cpg	654.03	J/molxK	810.06	Joback Method
cpg	665.80	J/molxK	841.09	Joback Method
cpg	676.82	J/molxK	872.11	Joback Method
dvisc	0.0019951	Paxs	380.51	Joback Method
dvisc	0.0009137	Paxs	431.42	Joback Method

dvisc	0.0004935	Paxs	482.33	Joback Method
dvisc	0.0002998	Paxs	533.24	Joback Method
dvisc	0.0001986	Paxs	584.15	Joback Method
dvisc	0.0001406	Paxs	635.06	Joback Method
dvisc	0.0001048	Paxs	685.97	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=U353539&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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