

Adipic acid, monochloride 2-methylpent-3-yl ester

Inchi:	InChI=1S/C12H21ClO3/c1-4-10(9(2)3)16-12(15)8-6-5-7-11(13)14/h9-10H,4-8H2,1-3H3
InchiKey:	JFCJPOAVRSQYAA-UHFFFAOYSA-N
Formula:	C12H21ClO3
SMILES:	CCC(OC(=O)CCCC(=O)Cl)C(C)C
Mol. weight [g/mol]:	248.75

Physical Properties

Property code	Value	Unit	Source
gf	-329.49	kJ/mol	Joback Method
hf	-674.69	kJ/mol	Joback Method
hfus	28.37	kJ/mol	Joback Method
hvap	61.82	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.290		Crippen Method
mvol	201.190	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1578.00		NIST Webbook
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tb	640.67	K	Joback Method
tc	828.94	K	Joback Method
tf	347.01	K	Joback Method
vc	0.774	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.39	J/molxK	640.67	Joback Method
cpg	533.93	J/molxK	672.05	Joback Method
cpg	547.74	J/molxK	703.43	Joback Method
cpg	560.83	J/molxK	734.81	Joback Method
cpg	573.20	J/molxK	766.19	Joback Method
cpg	584.88	J/molxK	797.57	Joback Method
cpg	595.87	J/molxK	828.94	Joback Method
dvisc	0.0032460	Paxs	347.01	Joback Method

dvisc	0.0014297	Paxs	395.95	Joback Method
dvisc	0.0007542	Paxs	444.90	Joback Method
dvisc	0.0004517	Paxs	493.84	Joback Method
dvisc	0.0002967	Paxs	542.78	Joback Method
dvisc	0.0002089	Paxs	591.73	Joback Method
dvisc	0.0001552	Paxs	640.67	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=U353574&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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