

Adipic acid, monochloride 3-hexyl ester

Inchi:	InChI=1S/C12H21ClO3/c1-3-7-10(4-2)16-12(15)9-6-5-8-11(13)14/h10H,3-9H2,1-2H3
InchiKey:	JXTRRRDOZBMDEB-UHFFFAOYSA-N
Formula:	C12H21ClO3
SMILES:	CCCC(CC)OC(=O)CCCCC(=O)Cl
Mol. weight [g/mol]:	248.75

Physical Properties

Property code	Value	Unit	Source
gf	-327.05	kJ/mol	Joback Method
hf	-669.41	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.434		Crippen Method
mcvol	201.190	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpola	1591.00		NIST Webbook
tb	641.11	K	Joback Method
tc	826.30	K	Joback Method
tf	362.01	K	Joback Method
vc	0.780	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.93	J/molxK	641.11	Joback Method
cpg	583.36	J/molxK	795.43	Joback Method
cpg	571.83	J/molxK	764.57	Joback Method
cpg	559.64	J/molxK	733.70	Joback Method
cpg	546.76	J/molxK	702.84	Joback Method
cpg	533.20	J/molxK	671.97	Joback Method
cpg	594.23	J/molxK	826.30	Joback Method
dvisc	0.0001669	Paxs	641.11	Joback Method
dvisc	0.0002200	Paxs	594.59	Joback Method

dvisc	0.0003039	Paxs	548.08	Joback Method
dvisc	0.0004458	Paxs	501.56	Joback Method
dvisc	0.0007072	Paxs	455.04	Joback Method
dvisc	0.0012461	Paxs	408.53	Joback Method
dvisc	0.0025398	Paxs	362.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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