

Glutaric acid, monochloride, trans-hex-3-enyl ester

Inchi:	InChI=1S/C11H17ClO3/c1-2-3-4-5-9-15-11(14)8-6-7-10(12)13/h3-4H,2,5-9H2,1H3/b4-3+
InchiKey:	QOVGVBWHKVYJJS-ONEGZZNKSA-N
Formula:	C11H17ClO3
SMILES:	CCC=CCCOC(=O)CCCC(=O)Cl
Mol. weight [g/mol]:	232.70

Physical Properties

Property code	Value	Unit	Source
gf	-252.81	kJ/mol	Joback Method
hf	-526.27	kJ/mol	Joback Method
hfus	33.03	kJ/mol	Joback Method
hvap	60.32	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.822		Crippen Method
mvol	182.800	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
tb	622.83	K	Joback Method
tc	813.33	K	Joback Method
tf	360.66	K	Joback Method
vc	0.711	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.69	J/molxK	622.83	Joback Method
cpg	459.56	J/molxK	654.58	Joback Method
cpg	471.76	J/molxK	686.33	Joback Method
cpg	483.33	J/molxK	718.08	Joback Method
cpg	494.27	J/molxK	749.83	Joback Method
cpg	504.61	J/molxK	781.58	Joback Method
cpg	514.37	J/molxK	813.33	Joback Method
dvisc	0.0020219	Paxs	360.66	Joback Method

dvisc	0.0010750	Paxs	404.36	Joback Method
dvisc	0.0006465	Paxs	448.05	Joback Method
dvisc	0.0004256	Paxs	491.75	Joback Method
dvisc	0.0003000	Paxs	535.44	Joback Method
dvisc	0.0002229	Paxs	579.13	Joback Method
dvisc	0.0001726	Paxs	622.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359939&Units=SI

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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