

Glutaric acid, monochloride, 2-ethylbutyl ester

Inchi:	InChI=1S/C11H19ClO3/c1-3-9(4-2)8-15-11(14)7-5-6-10(12)13/h9H,3-8H2,1-2H3
InchiKey:	QQIRYCRKMQJXDV-UHFFFAOYSA-N
Formula:	C11H19ClO3
SMILES:	CCC(CC)COC(=O)CCCC(=O)Cl
Mol. weight [g/mol]:	234.72

Physical Properties

Property code	Value	Unit	Source
gf	-335.47	kJ/mol	Joback Method
hf	-648.77	kJ/mol	Joback Method
hfus	29.31	kJ/mol	Joback Method
hvap	59.98	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.901		Crippen Method
mcvol	187.100	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinqol	1576.00		NIST Webbook
tb	618.23	K	Joback Method
tc	805.12	K	Joback Method
tf	350.74	K	Joback Method
vc	0.725	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.05	J/molxK	618.23	Joback Method
cpg	481.72	J/molxK	649.38	Joback Method
cpg	494.73	J/molxK	680.53	Joback Method
cpg	507.08	J/molxK	711.67	Joback Method
cpg	518.79	J/molxK	742.82	Joback Method
cpg	529.86	J/molxK	773.97	Joback Method
cpg	540.31	J/molxK	805.12	Joback Method
dvisc	0.0027334	Paxs	350.74	Joback Method
dvisc	0.0013605	Paxs	395.32	Joback Method

dvisc	0.0007801	Paxs	439.90	Joback Method
dvisc	0.0004955	Paxs	484.49	Joback Method
dvisc	0.0003397	Paxs	529.07	Joback Method
dvisc	0.0002470	Paxs	573.65	Joback Method
dvisc	0.0001880	Paxs	618.23	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=U359436&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
mccvol:	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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