Glutaric acid, monochloride, 2-hexyl ester

Inchi: InChI=1S/C11H19ClO3/c1-3-4-6-9(2)15-11(14)8-5-7-10(12)13/h9H,3-8H2,1-2H3
InchiKey: XFBCPFNWRIFUEL-UHFFFAOYSA-N
Formula: C11H19ClO3
SMILES: CCCCC(C)OC(=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	-3.33		Crippen Method
logp	3.044		Crippen Method
mcvol	187.100	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	1534.00		NIST Webbook
tb	618.23	K	Joback Method
tc	805.12	K	Joback Method
tf	350.74	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0007801	Pa×s	439.90	Joback Method
dvisc	0.0004955	Pa×s	484.49	Joback Method
dvisc	0.0003397	Pa×s	529.07	Joback Method
dvisc	0.0002470	Pa×s	573.65	Joback Method
dvisc	0.0001880	Pa×s	618.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359655&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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