

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

Inchi:	InChI=1S/C11H19ClO3/c1-4-9(8(2)3)15-11(14)7-5-6-10(12)13/h8-9H,4-7H2,1-3H3
InchiKey:	BPPSKCPYZOEKF-UHFFFAOYSA-N
Formula:	C11H19ClO3
SMILES:	CCC(OC(=O)CCCC(=O)Cl)C(C)C
Mol. weight [g/mol]:	234.72

Physical Properties

Property code	Value	Unit	Source
gf	-337.91	kJ/mol	Joback Method
hf	-654.05	kJ/mol	Joback Method
hfus	25.78	kJ/mol	Joback Method
hvap	59.59	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.900		Crippen Method
mvol	187.100	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1510.00		NIST Webbook
tb	617.79	K	Joback Method
tc	808.00	K	Joback Method
tf	335.74	K	Joback Method
vc	0.719	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.49	J/molxK	617.79	Joback Method
cpg	482.45	J/molxK	649.49	Joback Method
cpg	495.71	J/molxK	681.19	Joback Method
cpg	508.28	J/molxK	712.89	Joback Method
cpg	520.18	J/molxK	744.59	Joback Method
cpg	531.42	J/molxK	776.30	Joback Method
cpg	542.00	J/molxK	808.00	Joback Method
dvisc	0.0035275	Paxs	335.74	Joback Method

dvisc	0.0015730	Paxs	382.75	Joback Method
dvisc	0.0008370	Paxs	429.76	Joback Method
dvisc	0.0005044	Paxs	476.76	Joback Method
dvisc	0.0003329	Paxs	523.77	Joback Method
dvisc	0.0002352	Paxs	570.78	Joback Method
dvisc	0.0001753	Paxs	617.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359526&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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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