

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

Inchi:	InChI=1S/C10H17ClO3/c1-7(2)8(3)14-10(13)6-4-5-9(11)12/h7-8H,4-6H2,1-3H3
InchiKey:	PTTQIWUXFZAENE-UHFFFAOYSA-N
Formula:	C10H17ClO3
SMILES:	CC(C)C(C)OC(=O)CCCC(=O)Cl
Mol. weight [g/mol]:	220.69

Physical Properties

Property code	Value	Unit	Source
gf	-346.33	kJ/mol	Joback Method
hf	-633.41	kJ/mol	Joback Method
hfus	23.19	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.510		Crippen Method
mcvol	173.010	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1428.00		NIST Webbook
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tb	594.91	K	Joback Method
tc	787.34	K	Joback Method
tf	324.47	K	Joback Method
vc	0.662	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.12	J/mol×K	594.91	Joback Method
cpg	432.41	J/mol×K	626.98	Joback Method
cpg	445.04	J/mol×K	659.05	Joback Method
cpg	457.03	J/mol×K	691.12	Joback Method
cpg	468.38	J/mol×K	723.19	Joback Method
cpg	479.10	J/mol×K	755.26	Joback Method
cpg	489.20	J/mol×K	787.34	Joback Method
dvisc	0.0038044	Paxs	324.47	Joback Method

dvisc	0.0017189	Paxs	369.54	Joback Method
dvisc	0.0009231	Paxs	414.62	Joback Method
dvisc	0.0005600	Paxs	459.69	Joback Method
dvisc	0.0003714	Paxs	504.76	Joback Method
dvisc	0.0002635	Paxs	549.84	Joback Method
dvisc	0.0001969	Paxs	594.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359729&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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