

Glutaric acid, monochloride, neopentyl ester

Inchi:	InChI=1S/C10H17ClO3/c1-10(2,3)7-14-9(13)6-4-5-8(11)12/h4-7H2,1-3H3
InchiKey:	OIYIGOLXEBSCHQ-UHFFFAOYSA-N
Formula:	C10H17ClO3
SMILES:	CC(C)(C)COC(=O)CCCC(=O)Cl
Mol. weight [g/mol]:	220.69

Physical Properties

Property code	Value	Unit	Source
gf	-338.61	kJ/mol	Joback Method
hf	-631.60	kJ/mol	Joback Method
hfus	22.82	kJ/mol	Joback Method
hvap	56.84	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.511		Crippen Method
mcvol	173.010	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	1421.00		NIST Webbook
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tb	592.56	K	Joback Method
tc	787.99	K	Joback Method
tf	356.89	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.66	J/molxK	592.56	Joback Method
cpg	481.20	J/molxK	755.42	Joback Method
cpg	470.67	J/molxK	722.85	Joback Method
cpg	459.47	J/molxK	690.28	Joback Method
cpg	447.58	J/molxK	657.70	Joback Method
cpg	434.99	J/molxK	625.13	Joback Method
cpg	491.09	J/molxK	787.99	Joback Method
dvisc	0.0002022	Paxs	592.56	Joback Method

dvisc	0.0002657	Paxs	553.28	Joback Method
dvisc	0.0003639	Paxs	514.00	Joback Method
dvisc	0.0005251	Paxs	474.72	Joback Method
dvisc	0.0008096	Paxs	435.45	Joback Method
dvisc	0.0013601	Paxs	396.17	Joback Method
dvisc	0.0025613	Paxs	356.89	Joback Method

Sources

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=U358355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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