Dimethylmalonic acid, monochloride, neopentyl ester

Inchi: InChI=1S/C10H17ClO3/c1-9(2,3)6-14-8(13)10(4,5)7(11)12/h6H2,1-5H3
InchiKey: PLRQBCQJESPELA-UHFFFAOYSA-N
Formula: C10H17ClO3
SMILES: CC(C)(C)COC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]: 220.69

Physical Properties

Property code	Value	Unit	Source
gf	-335.77	kJ/mol	Joback Method
hf	-640.35	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	55.55	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.367		Crippen Method
mcvol	173.010	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	1174.00		NIST Webbook
tb	589.33	K	Joback Method
tc	795.95	K	Joback Method
tf	359.31	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.03	J/mol×K	589.33	Joback Method
cpg	439.07	J/mol×K	623.77	Joback Method
cpg	452.20	J/mol×K	658.20	Joback Method
cpg	464.46	J/mol×K	692.64	Joback Method
cpg	475.91	J/mol×K	727.08	Joback Method
cpg	486.58	J/mol×K	761.51	Joback Method
cpg	496.52	J/mol×K	795.95	Joback Method
dvisc	0.0028093	Pa×s	359.31	Joback Method
dvisc	0.0014292	Pa×s	397.65	Joback Method

dvisc	0.0008188	Pa×s	435.98	Joback Method
dvisc	0.0005133	Pa×s	474.32	Joback Method
dvisc	0.0003451	Pa×s	512.66	Joback Method
dvisc	0.0002452	Pa×s	550.99	Joback Method
dvisc	0.0001821	Pa×s	589.33	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361760&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

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