Methylcamphonanate

Inchi: InChI=1S/C10H14O4/c1-9(2)6-4-5-10(9,8(12)13-3)14-7(6)11/h6H,4-5H2,1-3H3/t6-,10+/m
InchiKey: YRCMNXAYMWJRKK-QUBYGPBYSA-N
Formula: C10H14O4
SMILES: COC(=O)C12CCC(C(=O)O1)C2(C)C
Mol. weight [g/mol]: 198.22

Physical Properties

Property code	Value	Unit	Source
gf	-318.60	kJ/mol	Joback Method
hf	-614.65	kJ/mol	Joback Method
hfus	14.58	kJ/mol	Joback Method
hvap	53.15	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.891		Crippen Method
mcvol	144.920	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1105.00		NIST Webbook
tb	612.82	K	Joback Method
tc	847.84	K	Joback Method
tf	445.33	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.65	J/mol×K	612.82	Joback Method
cpg	414.85	J/mol×K	651.99	Joback Method
cpg	429.30	J/mol×K	691.16	Joback Method
cpg	443.22	J/mol×K	730.33	Joback Method
cpg	456.86	J/mol×K	769.50	Joback Method
cpg	470.45	J/mol×K	808.67	Joback Method
cpg	484.23	J/mol×K	847.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229311&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
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