Methylmyrtenate

Inchi: InChI=1S/C11H16O2/c1-11(2)7-4-5-8(9(11)6-7)10(12)13-3/h5,7,9H,4,6H2,1-3H3
InchiKey: HBIHNNBZGOVTTR-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: COC(=O)C1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 180.24
CAS: 30649-97-9

Physical Properties

Property code	Value	Unit	Source
gf	-75.65	kJ/mol	Joback Method
hf	-334.52	kJ/mol	Joback Method
hfus	16.81	kJ/mol	Joback Method
hvap	48.73	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.152		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1282.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1301.30		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1301.30		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1670.00		NIST Webbook
tb	544.83	K	Joback Method
tc	758.79	K	Joback Method
tf	351.19	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.41	J/mol×K	544.83	Joback Method

cpg	386.76	J/mol×K	580.49	Joback Method
cpg	402.06	J/mol×K	616.15	Joback Method
cpg	416.45	J/mol×K	651.81	Joback Method
cpg	430.05	J/mol×K	687.47	Joback Method
cpg	442.98	J/mol×K	723.13	Joback Method
cpg	455.39	J/mol×K	758.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30649979&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume