Myrcenyl propionate

Inchi: InChI=1S/C13H22O2/c1-6-11(3)9-8-10-13(4,5)15-12(14)7-2/h6H,1,3,7-10H2,2,4-5H3
InchiKey: RGLNFSSMFMUBER-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: C=CC(=C)CCCC(C)(C)OC(=O)CC
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-5.37	kJ/mol	Joback Method
hf	-324.13	kJ/mol	Joback Method
hfus	20.93	kJ/mol	Joback Method
hvap	51.13	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.631		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	1327.00		NIST Webbook
rinpol	1327.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1625.00		NIST Webbook
tb	563.14	K	Joback Method
tc	749.53	K	Joback Method
tf	293.37	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.61	J/mol×K	563.14	Joback Method
cpg	492.99	J/mol×K	594.21	Joback Method
cpg	508.52	J/mol×K	625.27	Joback Method
cpg	523.23	J/mol×K	656.34	Joback Method
cpg	537.17	J/mol×K	687.40	Joback Method
cpg	550.37	J/mol×K	718.47	Joback Method

cpg	562.85	J/mol×K	749.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410087&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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