Myrcen-8-yl acetate

Inchi: InChI=1S/C12H18O2/c1-5-10(2)7-6-8-11(3)9-14-12(4)13/h5,8H,1-2,6-7,9H2,3-4H3/b11-8
InchiKey: YGUUXLXMTKARJN-DHZHZOJOSA-N
Formula: C12H18O2
SMILES: C=CC(=C)CCC=C(C)COC(C)=O
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	55.04	kJ/mol	Joback Method
hf	-187.31	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	50.24	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.018		Crippen Method
mcvol	174.480	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1348.00		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1737.00		NIST Webbook
tb	547.53	K	Joback Method
tc	736.56	K	Joback Method
tf	260.64	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.87	J/mol×K	547.53	Joback Method
cpg	420.52	J/mol×K	579.03	Joback Method
cpg	434.44	J/mol×K	610.54	Joback Method
cpg	447.66	J/mol×K	642.04	Joback Method
cpg	460.22	J/mol×K	673.55	Joback Method
cpg	472.12	J/mol×K	705.05	Joback Method

cpg	483.42	J/mol×K	736.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R611339&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

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