Allyl ionone 3

Inchi: InChI=1S/C16H24O/c1-5-6-9-14(17)10-11-15-13(2)8-7-12-16(15,3)4/h5,8,10-11,15H,1,6-
InchiKey: FXCYGAGBPZQRJE-ZHACJKMWSA-N
Formula: C16H24O
SMILES: C=CCCC(=O)C=CC1C(C)=CCCC1(C)C
Mol. weight [g/mol]: 232.36

Physical Properties

Property code	Value	Unit	Source
gf	154.56	kJ/mol	Joback Method
hf	-147.97	kJ/mol	Joback Method
hfus	25.16	kJ/mol	Joback Method
hvap	57.17	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.460		Crippen Method
mcvol	214.110	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
ripol	2146.00		NIST Webbook
ripol	2146.00		NIST Webbook
tb	639.45	K	Joback Method
tc	850.87	K	Joback Method
tf	353.49	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.70	J/mol×K	639.45	Joback Method
cpg	592.10	J/mol×K	674.69	Joback Method
cpg	610.47	J/mol×K	709.92	Joback Method
cpg	627.94	J/mol×K	745.16	Joback Method
cpg	644.64	J/mol×K	780.40	Joback Method
cpg	660.70	J/mol×K	815.63	Joback Method

cpg	676.26	J/mol×K	850.87	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=U284929&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

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