Myrtenyl hexanoate

Inchi: InChI=1S/C16H26O2/c1-4-5-6-7-15(17)18-11-12-8-9-13-10-14(12)16(13,2)3/h8,13-14H,4
InchiKey: TWSZIXSQUCWBEC-UHFFFAOYSA-N
Formula: C16H26O2
SMILES: CCCCCC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	-33.55	kJ/mol	Joback Method
hf	-437.72	kJ/mol	Joback Method
hfus	29.76	kJ/mol	Joback Method
hvap	59.86	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.102		Crippen Method
mcvol	217.720	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1640.00		NIST Webbook
rinpol	1640.00		NIST Webbook
tb	659.23	K	Joback Method
tc	857.82	K	Joback Method
tf	407.54	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.77	J/mol×K	659.23	Joback Method
cpg	645.53	J/mol×K	692.33	Joback Method
cpg	663.41	J/mol×K	725.43	Joback Method
cpg	680.52	J/mol×K	758.53	Joback Method
cpg	696.99	J/mol×K	791.62	Joback Method
cpg	712.93	J/mol×K	824.72	Joback Method
cpg	728.46	J/mol×K	857.82	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=R224970&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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