Myraldyl acetate 1

Inchi: InChI=1S/C15H24O2/c1-12(2)6-4-7-14-8-5-9-15(10-14)11-17-13(3)16/h6,8,15H,4-5,7,9-1
InchiKey: IIUKCYITROTKFB-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: CC(=O)OCC1CCC=C(CCC=C(C)C)C1
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-42.05	kJ/mol	Joback Method
hf	-389.67	kJ/mol	Joback Method
hfus	28.95	kJ/mol	Joback Method
hvap	59.56	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.022		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	1704.00		NIST Webbook
rinpol	1682.90		NIST Webbook
ripol	2199.00		NIST Webbook
ripol	2166.00		NIST Webbook
tb	646.62	K	Joback Method
tc	851.38	K	Joback Method
tf	332.59	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.56	J/mol×K	646.62	Joback Method
cpg	590.53	J/mol×K	680.75	Joback Method
cpg	608.43	J/mol×K	714.87	Joback Method
cpg	625.29	J/mol×K	749.00	Joback Method
cpg	641.15	J/mol×K	783.13	Joback Method
cpg	656.03	J/mol×K	817.26	Joback Method

cpg	669.97	J/mol×K	851.38	Joback Method

Sources

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=R185865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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