

Lavandulyl propionate

Inchi: InChI=1S/C13H22O2/c1-6-13(14)15-9-12(11(4)5)8-7-10(2)3/h12H,2,4,6-9H2,1,3,5H3
InchiKey: MUZPKOFBDLINTJ-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: C=C(C)CCC(COC(=O)CC)C(=C)C
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
hfus	23.51	kJ/mol	Joback Method
hvap	66.82	kJ/mol	Cheméo Relay (1.0)
ie	9.04	eV	Cheméo Relay (1.0)
logp	3.488		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1364.00		NIST Webbook
rinpol	1364.00		NIST Webbook
tb	518.67	K	Cheméo Relay (1.0)
tc	685.15	K	Cheméo Relay (1.0)
tf	220.93	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.71	J/mol×K	565.81	Joback Method
cpg	489.77	J/mol×K	596.31	Joback Method
cpg	505.10	J/mol×K	626.81	Joback Method
cpg	519.71	J/mol×K	657.32	Joback Method
cpg	533.62	J/mol×K	687.82	Joback Method
cpg	546.85	J/mol×K	718.32	Joback Method
cpg	559.42	J/mol×K	748.82	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232807&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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