

Menthyl lactate

Inchi:	InChI=1S/C13H24O3/c1-8(2)11-6-5-9(3)7-12(11)16-13(15)10(4)14/h8-12,14H,5-7H2,1-4H
InchiKey:	UJNOLBSYLSYIBM-BEZGRXCVSA-N
Formula:	C13H24O3
SMILES:	CC1CCC(C(C)C)C(OC(=O)C(C)O)C1
Mol. weight [g/mol]:	228.33

Physical Properties

Property code	Value	Unit	Source
gf	-308.01	kJ/mol	Joback Method
hf	-705.60	kJ/mol	Joback Method
hfus	23.23	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.371		Crippen Method
mcvol	196.480	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1473.00		NIST Webbook
tb	674.64	K	Joback Method
tc	867.50	K	Joback Method
tf	338.15	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.51	J/molxK	674.64	Joback Method
cpg	659.85	J/molxK	835.36	Joback Method
cpg	646.10	J/molxK	803.21	Joback Method
cpg	631.40	J/molxK	771.07	Joback Method
cpg	615.74	J/molxK	738.93	Joback Method
cpg	599.12	J/molxK	706.78	Joback Method
cpg	672.66	J/molxK	867.50	Joback Method
dvisc	0.0000568	Paxs	674.64	Joback Method
dvisc	0.0000888	Paxs	618.56	Joback Method

dvisc	0.0001519	Paxs	562.48	Joback Method
dvisc	0.0002924	Paxs	506.39	Joback Method
dvisc	0.0006627	Paxs	450.31	Joback Method
dvisc	0.0018956	Paxs	394.23	Joback Method
dvisc	0.0076841	Paxs	338.15	Joback Method

Sources

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=R199938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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