«beta»-Citronellol, methyl ether

Other names: Methyl citronellol
Inchi: InChI=1S/C11H22O/c1-10(2)6-5-7-11(3)8-9-12-4/h6,11H,5,7-9H2,1-4H3
InchiKey: QUGQATRJSUHGGA-UHFFFAOYSA-N
Formula: C11H22O
SMILES: COCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 170.29

Physical Properties

Property code	Value	Unit	Source
gf	5.97	kJ/mol	Joback Method
hf	-300.44	kJ/mol	Joback Method
hfus	20.80	kJ/mol	Joback Method
hvap	42.14	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.405		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1174.70		NIST Webbook
rinpol	1174.70		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1540.00		NIST Webbook
tb	477.10	K	Joback Method
tc	652.55	K	Joback Method
tf	201.92	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.89	J/mol×K	477.10	Joback Method
cpg	387.98	J/mol×K	506.34	Joback Method
cpg	403.42	J/mol×K	535.58	Joback Method

cpg	418.22	J/mol×K	564.82	Joback Method
cpg	432.41	J/mol×K	594.07	Joback Method
cpg	446.00	J/mol×K	623.31	Joback Method
cpg	459.00	J/mol×K	652.55	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=U333814&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
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