.ALPHA.-LINALOOL

Other names: «alpha»-Linalool
3,7-dimethyl-1,7-octadien-3-ol
Inchi: InChI=1S/C10H18O/c1-5-10(4,11)8-6-7-9(2)3/h5,11H,1-2,6-8H2,3-4H3
InchiKey: GYJHTGZQPKPEOT-UHFFFAOYSA-N
Formula: C10H18O
SMILES: C=CC(C)(O)CCCC(=C)C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
hfus	14.46	kJ/mol	Joback Method
hvap	62.22	kJ/mol	Cheméo Relay (1.0)
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-1.81		Cheméo Relay (1.0)
logp	2.670		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
rinpol	1098.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1098.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1564.00		NIST Webbook
tb	462.02	K	Cheméo Relay (1.0)
tc	649.49	K	Cheméo Relay (1.0)
tf	261.98	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.21	J/mol×K	510.39	Joback Method
cpg	359.42	J/mol×K	539.64	Joback Method
cpg	371.94	J/mol×K	568.89	Joback Method

cpg	383.79	J/mol×K	598.14	Joback Method
cpg	395.03	J/mol×K	627.39	Joback Method
cpg	405.67	J/mol×K	656.64	Joback Method
cpg	415.75	J/mol×K	685.90	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C598072&Units=SI

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):

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

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