(E)-Myroxide

Other names: trans-myroxide
Inchi: InChI=1S/C10H16O/c1-5-8(2)6-7-9-10(3,4)11-9/h5-6,9H,1,7H2,2-4H3/b8-6+
InchiKey: LIMXJCIGROLRED-SOFGYWHQSA-N
Formula: C10H16O
SMILES: C=CC(C)=CCC1OC1(C)C
Mol. weight [g/mol]: 152.23
CAS: 94607-47-3

Physical Properties

Property code	Value	Unit	Source
gf	154.26	kJ/mol	Joback Method
hf	-81.17	kJ/mol	Joback Method
hfus	20.15	kJ/mol	Joback Method
hvap	40.19	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.686		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1142.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1136.00		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1484.00		NIST Webbook
tb	458.18	K	Joback Method
tc	657.47	K	Joback Method
tf	245.83	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.19	J/mol×K	458.18	Joback Method
cpg	318.21	J/mol×K	491.40	Joback Method
cpg	333.07	J/mol×K	524.61	Joback Method
cpg	346.90	J/mol×K	557.83	Joback Method
cpg	359.80	J/mol×K	591.04	Joback Method
cpg	371.90	J/mol×K	624.26	Joback Method
cpg	383.32	J/mol×K	657.47	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=C94607473&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

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