Bicyclo[2.2.1]heptane, 2-methoxy-1,7,7-trimethyl-

Other names: 2-Methoxy-1,7,7-trimethylbicyclo[2.2.1]heptane
Inchi: InChI=1S/C11H20O/c1-10(2)8-5-6-11(10,3)9(7-8)12-4/h8-9H,5-7H2,1-4H3
InchiKey: ZRHVOKYSOWTPIG-UHFFFAOYSA-N
Formula: C11H20O
SMILES: COC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]: 168.28
CAS: 4443-51-0

Physical Properties

Property code	Value	Unit	Source
gf	19.74	kJ/mol	Joback Method
hf	-273.35	kJ/mol	Joback Method
hfus	9.15	kJ/mol	Joback Method
hvap	39.57	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.848		Crippen Method
mcvol	150.000	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1116.60		NIST Webbook
rinpol	1116.60		NIST Webbook
tb	482.39	K	Joback Method
tc	692.35	K	Joback Method
tf	307.64	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.31	J/mol×K	482.39	Joback Method
cpg	382.50	J/mol×K	517.38	Joback Method
cpg	401.19	J/mol×K	552.38	Joback Method
cpg	418.58	J/mol×K	587.37	Joback Method
cpg	434.87	J/mol×K	622.36	Joback Method
cpg	450.26	J/mol×K	657.36	Joback Method

cpg	464.95	J/mol×K	692.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C4443510&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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