Nerol, methyl ether

Inchi: InChI=1S/C11H20O/c1-10(2)6-5-7-11(3)8-9-12-4/h6,8H,5,7,9H2,1-4H3/b11-8-
InchiKey: AVJMJMPVWWWELJ-FLIBITNWSA-N
Formula: C11H20O
SMILES: COCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 168.28

Physical Properties

Property code	Value	Unit	Source
gf	80.08	kJ/mol	Joback Method
hf	-187.73	kJ/mol	Joback Method
hfus	23.22	kJ/mol	Joback Method
hvap	42.57	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.325		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1211.90		NIST Webbook
tb	481.58	K	Joback Method
tc	664.47	K	Joback Method
tf	197.88	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.28	J/mol×K	481.58	Joback Method
cpg	370.97	J/mol×K	512.06	Joback Method
cpg	385.94	J/mol×K	542.54	Joback Method
cpg	400.23	J/mol×K	573.03	Joback Method
cpg	413.85	J/mol×K	603.51	Joback Method
cpg	426.85	J/mol×K	633.99	Joback Method
cpg	439.23	J/mol×K	664.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352641&Units=SI
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

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