

Myrtenyl methyl ether

Inchi:	InChI=1S/C11H18O/c1-11(2)9-5-4-8(7-12-3)10(11)6-9/h4,9-10H,5-7H2,1-3H3
InchiKey:	GMIAZJHVKQKHSD-UHFFFAOYSA-N
Formula:	C11H18O
SMILES:	COCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]:	166.26
CAS:	202527-57-9

Physical Properties

Property code	Value	Unit	Source
gf	53.27	kJ/mol	Joback Method
hf	-221.94	kJ/mol	Joback Method
hfus	15.21	kJ/mol	Joback Method
hvap	41.98	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.625		Crippen Method
mvol	145.700	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1160.50		NIST Webbook
ripol	1372.00		NIST Webbook
tb	490.96	K	Joback Method
tc	695.76	K	Joback Method
tf	301.26	K	Joback Method
vc	0.558	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.39	J/mol×K	490.96	Joback Method
cpg	364.36	J/mol×K	525.09	Joback Method
cpg	381.18	J/mol×K	559.23	Joback Method
cpg	396.96	J/mol×K	593.36	Joback Method
cpg	411.81	J/mol×K	627.49	Joback Method
cpg	425.86	J/mol×K	661.62	Joback Method
cpg	439.22	J/mol×K	695.76	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=C202527579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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