Khusian-2-yl methyl ether

Inchi: InChI=1S/C16H28O/c1-11-6-7-12-14(2,3)15(4)8-9-16(11,12)10-13(15)17-5/h11-13H,6-10
InchiKey: HZXKFYFDUDQEAJ-LTAXLKKJSA-N
Formula: C16H28O
SMILES: COC1CC23CCC1(C)C(C)(C)C2CCC3C
Mol. weight [g/mol]: 236.39

Physical Properties

Property code	Value	Unit	Source
gf	97.29	kJ/mol	Joback Method
hf	-315.01	kJ/mol	Joback Method
hfus	12.91	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.264		Crippen Method
mcvol	209.590	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1600.00		NIST Webbook
ripol	1860.00		NIST Webbook
tb	603.37	K	Joback Method
tc	827.45	K	Joback Method
tf	398.07	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.75	J/mol×K	603.37	Joback Method
cpg	629.98	J/mol×K	640.72	Joback Method
cpg	652.85	J/mol×K	678.06	Joback Method
cpg	674.75	J/mol×K	715.41	Joback Method
cpg	696.04	J/mol×K	752.76	Joback Method
cpg	717.07	J/mol×K	790.11	Joback Method
cpg	738.23	J/mol×K	827.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R236265&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume