

Cyclocopacamphan-12-yl methyl ether, B

Inchi:	InChI=1S/C16H24O2/c1-8(14(17)18-4)9-5-6-15(2)10-7-11-13(12(9)10)16(11,15)3/h8-13H
InchiKey:	IRQZAMHHIOKADI-UZXMILTCSA-N
Formula:	C16H24O2
SMILES:	COC(=O)C(C)C1CCC2(C)C3CC4C(C13)C42C
Mol. weight [g/mol]:	248.36

Physical Properties

Property code	Value	Unit	Source
gf	80.57	kJ/mol	Joback Method
hf	-350.67	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	56.06	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	3.114		Crippen Method
mvol	200.300	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	1583.00		NIST Webbook
rinpol	1583.00		NIST Webbook
tb	646.22	K	Joback Method
tc	859.88	K	Joback Method
tf	441.12	K	Joback Method
vc	0.786	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.24	J/molxK	646.22	Joback Method
cpg	634.03	J/molxK	681.83	Joback Method
cpg	652.86	J/molxK	717.44	Joback Method
cpg	671.03	J/molxK	753.05	Joback Method
cpg	688.84	J/molxK	788.66	Joback Method
cpg	706.56	J/molxK	824.27	Joback Method
cpg	724.51	J/molxK	859.88	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=R236161&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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