Cyclocopacamphan-12-yl methyl ether, epimer b

Inchi: InChI=1S/C16H26O/c1-9(8-17-4)10-5-6-15(2)11-7-12-14(13(10)11)16(12,15)3/h9-14H,5-

InchiKey: GPTFZPFEBLBCNT-HIMZGLRWSA-N

Formula: C16H26O

SMILES: COCC(C)C1CCC2(C)C3CC4C(C13)C42C

Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	209.49	kJ/mol	Joback Method
hf	-238.09	kJ/mol	Joback Method
hfus	22.22	kJ/mol	Joback Method
hvap	49.31	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.587		Crippen Method
mcvol	198.730	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	1583.00		NIST Webbook
rinpol	1583.00		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1849.00		NIST Webbook
tb	592.35	K	Joback Method
tc	798.96	K	Joback Method
tf	391.19	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.38	J/mol×K	592.35	Joback Method
cpg	608.00	J/mol×K	626.79	Joback Method
cpg	628.31	J/mol×K	661.22	Joback Method
cpg	647.55	J/mol×K	695.66	Joback Method
cpg	666.01	J/mol×K	730.09	Joback Method
cpg	683.95	J/mol×K	764.53	Joback Method

cpg	701.64	J/mol×K	798.96	Joback Method

Sources

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=R397885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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