

Copaborneol

Inchi: InChI=1S/C16H28O/c1-10(2)11-5-7-15(3)13-6-8-16(15,4)14(17)12(13)9-11/h10-14,17H,5
InchiKey: QZNBJJCJJAQRMJ-WSQROMCKSA-N
Formula: C16H28O
SMILES: CC(C)C1CCC2(C)C3CCC2(C)C(O)C3C1
Mol. weight [g/mol]: 236.39

Physical Properties

Property code	Value	Unit	Source
gf	68.52	kJ/mol	Joback Method
hf	-355.54	kJ/mol	Joback Method
hfus	18.58	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.856		Crippen Method
mcvol	209.590	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1601.00		NIST Webbook
ripol	2142.00		NIST Webbook
ripol	2142.00		NIST Webbook
tb	672.45	K	Joback Method
tc	879.43	K	Joback Method
tf	397.76	K	Joback Method
vc	0.792	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.94	J/molxK	672.45	Joback Method
cpg	675.74	J/molxK	706.95	Joback Method
cpg	695.69	J/molxK	741.44	Joback Method

cpg	715.02	J/mol×K	775.94	Joback Method
cpg	733.96	J/mol×K	810.44	Joback Method
cpg	752.75	J/mol×K	844.94	Joback Method
cpg	771.60	J/mol×K	879.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R615262&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

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