

carissone

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C15H24O2/c1-10-12-9-11(14(2,3)17)5-7-15(12,4)8-6-13(10)16/h11,17H,5-9H2

ZWSWPQHKDLIDL-UHFFFAOYSA-N

C15H24O2

CC1=C2CC(C(C)(C)O)CCC2(C)CCC1=O

236.35

473-10-9

Physical Properties

Property code	Value	Unit	Source
gf	-102.84	kJ/mol	Joback Method
hf	-480.57	kJ/mol	Joback Method
hfus	12.81	kJ/mol	Joback Method
hvap	69.59	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.243		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1883.00		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	1935.70		NIST Webbook
rinpol	1922.00		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1935.70		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1895.00		NIST Webbook
ripol	2627.00		NIST Webbook
tb	739.29	K	Joback Method
tc	963.16	K	Joback Method
tf	461.77	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	631.75	J/mol×K	739.29	Joback Method
cpg	650.32	J/mol×K	776.60	Joback Method
cpg	668.06	J/mol×K	813.91	Joback Method
cpg	685.09	J/mol×K	851.23	Joback Method
cpg	701.58	J/mol×K	888.54	Joback Method
cpg	717.66	J/mol×K	925.85	Joback Method
cpg	733.49	J/mol×K	963.16	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=C473109&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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