

7,10-Epoxy-10-methoxysalvialane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C16H28O2/c1-11(2)12-6-7-15(4)13(12)10-14(3)8-9-16(15,17-5)18-14/h11-13H

XQLGIQDOQAKOHV-AKJSJKFASA-N

C16H28O2

COC12CCC(C)(CC3C(C(C)C)CCC31C)O2

252.39

Physical Properties

Property code	Value	Unit	Source
gf	16.44	kJ/mol	Joback Method
hf	-431.95	kJ/mol	Joback Method
hfus	16.29	kJ/mol	Joback Method
hvap	53.75	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.990		Crippen Method
mcvol	215.460	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1586.00		NIST Webbook
tb	634.55	K	Joback Method
tc	860.66	K	Joback Method
tf	413.88	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.29	J/mol×K	634.55	Joback Method
cpg	664.39	J/mol×K	672.24	Joback Method
cpg	686.42	J/mol×K	709.92	Joback Method
cpg	707.76	J/mol×K	747.61	Joback Method
cpg	728.79	J/mol×K	785.29	Joback Method
cpg	749.89	J/mol×K	822.98	Joback Method
cpg	771.45	J/mol×K	860.66	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=R236101&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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