

Drim-8-en-7-one

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24O/c1-10-11(2)15(5)8-6-7-14(3,4)13(15)9-12(10)16/h13H,6-9H2,1-5H3

VEEZSMVXABVRFI-UHFFFAOYSA-N

C15H24O

CC1=C(C)C2(C)CCCC(C)(C)C2CC1=O

220.35

Physical Properties

Property code	Value	Unit	Source
gf	17.94	kJ/mol	Joback Method
hf	-324.69	kJ/mol	Joback Method
hfus	10.90	kJ/mol	Joback Method
hvap	52.75	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.128		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1763.00		NIST Webbook
rinpol	1763.00		NIST Webbook
tb	645.91	K	Joback Method
tc	884.64	K	Joback Method
tf	418.19	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.93	J/mol×K	645.91	Joback Method
cpg	582.21	J/mol×K	685.70	Joback Method
cpg	603.48	J/mol×K	725.49	Joback Method
cpg	623.99	J/mol×K	765.28	Joback Method
cpg	643.99	J/mol×K	805.07	Joback Method
cpg	663.73	J/mol×K	844.86	Joback Method
cpg	683.46	J/mol×K	884.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229193&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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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