

Kelsoene

Inchi: InChI=1S/C15H24/c1-9(2)13-12-7-8-15(12,4)11-6-5-10(3)14(11)13/h10-14H,1,5-8H2,2-4
InchiKey: UEHKTJFOLYEULK-QZDKWAGWSA-N
Formula: C15H24
SMILES: C=C(C)C1C2C(C)CCC2C2(C)CCC12
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	296.24	kJ/mol	Joback Method
hf	-70.83	kJ/mol	Joback Method
hfus	21.24	kJ/mol	Joback Method
hvap	46.23	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpola	1420.00		NIST Webbook
rinpola	1420.00		NIST Webbook
tb	549.88	K	Joback Method
tc	764.29	K	Joback Method
tf	304.57	K	Joback Method
vc	0.716	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.04	J/mol×K	549.88	Joback Method
cpg	524.93	J/mol×K	585.62	Joback Method
cpg	547.24	J/mol×K	621.35	Joback Method
cpg	568.12	J/mol×K	657.09	Joback Method
cpg	587.78	J/mol×K	692.82	Joback Method
cpg	606.40	J/mol×K	728.56	Joback Method
cpg	624.15	J/mol×K	764.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R412741&Units=SI

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

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