

bulnesene

Inchi:	InChI=1S/C15H26/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h10,12-13,15H,5-9H2,1-
InchiKey:	AAPYGFMEZRXPJI-VNHYZAJKSA-N
Formula:	C15H26
SMILES:	CC1=C2CCC(C)C2CC(C(C)C)CC1
Mol. weight [g/mol]:	206.37

Physical Properties

Property code	Value	Unit	Source
gf	149.07	kJ/mol	Joback Method
hf	-222.75	kJ/mol	Joback Method
hfus	20.47	kJ/mol	Joback Method
hvap	50.42	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.805		Crippen Method
mcvol	196.190	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
tb	577.17	K	Joback Method
tc	790.56	K	Joback Method
tf	287.17	K	Joback Method
vc	0.737	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.34	J/molxK	577.17	Joback Method
cpg	629.55	J/molxK	755.00	Joback Method
cpg	610.82	J/molxK	719.43	Joback Method
cpg	590.87	J/molxK	683.87	Joback Method
cpg	569.68	J/molxK	648.30	Joback Method
cpg	547.18	J/molxK	612.74	Joback Method
cpg	647.13	J/molxK	790.56	Joback Method
dvisc	0.0003337	Paxs	577.17	Joback Method

dvisc	0.0003995	Paxs	528.84	Joback Method
dvisc	0.0004959	Paxs	480.50	Joback Method
dvisc	0.0006461	Paxs	432.17	Joback Method
dvisc	0.0008997	Paxs	383.84	Joback Method
dvisc	0.0013783	Paxs	335.50	Joback Method
dvisc	0.0024375	Paxs	287.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407813&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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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