

«alpha»-panasinsen

Inchi:	InChI=1S/C15H24/c1-11-6-5-8-14(4)9-7-12-13(2,3)10-15(11,12)14/h6,12H,5,7-10H2,1-4H
InchiKey:	WHXUZXDWQKUIJL-VHDGCEQUSA-N
Formula:	C15H24
SMILES:	CC1=CCCC2(C)CCC3C(C)(C)CC132
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	229.62	kJ/mol	Joback Method
hf	-75.16	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
ripol	1840.00		NIST Webbook
ripol	1840.00		NIST Webbook
tb	571.55	K	Joback Method
tc	806.48	K	Joback Method
tf	386.33	K	Joback Method
vc	0.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.53	J/mol×K	571.55	Joback Method
cpg	523.86	J/mol×K	610.71	Joback Method
cpg	544.56	J/mol×K	649.86	Joback Method
cpg	564.09	J/mol×K	689.02	Joback Method
cpg	582.88	J/mol×K	728.17	Joback Method
cpg	601.40	J/mol×K	767.33	Joback Method
cpg	620.08	J/mol×K	806.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333618&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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