

Panaxene

Inchi:	InChI=1S/C15H24/c1-7-14(6)9-8-12-13(4,5)10-15(12,14)11(2)3/h7,12H,1-2,8-10H2,3-6H
InchiKey:	UAOBSVDFJSNTLJ-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	<chem>C=CC1(C)CCC2C(C)(C)CC21C(=C)C</chem>
Mol. weight [g/mol]:	204.35
CAS:	871660-95-6

Physical Properties

Property code	Value	Unit	Source
gf	320.06	kJ/mol	Joback Method
hf	32.62	kJ/mol	Joback Method
hfus	8.15	kJ/mol	Joback Method
hvap	43.65	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1312.00		NIST Webbook
rinpol	1313.60		NIST Webbook
rinpol	1313.60		NIST Webbook
tb	544.97	K	Joback Method
tc	765.66	K	Joback Method
tf	336.91	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.98	J/molxK	544.97	Joback Method
cpg	513.69	J/molxK	581.75	Joback Method
cpg	533.75	J/molxK	618.53	Joback Method
cpg	552.52	J/molxK	655.31	Joback Method
cpg	570.37	J/molxK	692.10	Joback Method
cpg	587.65	J/molxK	728.88	Joback Method

Sources

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=C871660956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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