

Calarenepoxide

Other names:	[1R-(1«alpha»,3a«beta»,4aR*,6a«alpha»,7a«alpha»,7b«alpha»)]-decahydro-1,7,7,7b-te
Inchi:	InChI=1S/C15H24O/c1-9-5-6-11-15(16-11)8-7-10-12(13(10,2)3)14(9,15)4/h9-12H,5-8H2,
InchiKey:	UYPPHUAQDGVVKN-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC1CCC2OC23CCC2C(C2(C)C)C13C
Mol. weight [g/mol]:	220.35
CAS:	68926-75-0

Physical Properties

Property code	Value	Unit	Source
gf	192.70	kJ/mol	Joback Method
hf	-209.03	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	48.77	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.626		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1592.00		NIST Webbook
tb	583.22	K	Joback Method
tc	812.69	K	Joback Method
tf	416.12	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.98	J/molxK	583.22	Joback Method
cpg	563.50	J/molxK	621.46	Joback Method
cpg	584.43	J/molxK	659.71	Joback Method
cpg	604.21	J/molxK	697.95	Joback Method
cpg	623.32	J/molxK	736.20	Joback Method
cpg	642.20	J/molxK	774.44	Joback Method
cpg	661.33	J/molxK	812.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68926750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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