

Erythrodiene

Inchi: InChI=1S/C15H24/c1-11(2)14-8-7-13(4)15(10-14)9-5-6-12(15)3/h11,14H,3-10H2,1-2H3/t
InchiKey: WKUVNTPZIMJKBY-GICMACPYSA-N
Formula: C15H24
SMILES: C=C1CCCC12CC(C(C)C)CCC2=C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	246.75	kJ/mol	Joback Method
hf	-53.53	kJ/mol	Joback Method
hfus	10.34	kJ/mol	Joback Method
hvap	48.28	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1447.00		NIST Webbook
tb	571.28	K	Joback Method
tc	792.87	K	Joback Method
tf	316.87	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.09	J/mol×K	571.28	Joback Method
cpg	520.73	J/mol×K	608.21	Joback Method
cpg	541.97	J/mol×K	645.14	Joback Method
cpg	561.96	J/mol×K	682.08	Joback Method
cpg	580.85	J/mol×K	719.01	Joback Method
cpg	598.78	J/mol×K	755.94	Joback Method
cpg	615.91	J/mol×K	792.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R428994&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
hvac:	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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