

Zierene

Inchi: InChI=1S/C15H24/c1-10(2)13-7-5-6-11(3)14-9-8-12(4)15(13)14/h10,13-15H,3-9H2,1-2H3
InchiKey: XXYZAUXDDZGORP-QLFBSQMISA-N
Formula: C15H24
SMILES: C=C1CCCC(C(C)C)C2C(=C)CCC12
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	244.53	kJ/mol	Joback Method
hf	-89.11	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinqol	1473.00		NIST Webbook
tb	566.37	K	Joback Method
tc	779.32	K	Joback Method
tf	288.73	K	Joback Method
vc	0.719	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.92	J/molxK	566.37	Joback Method
cpg	523.12	J/molxK	601.86	Joback Method
cpg	545.00	J/molxK	637.35	Joback Method
cpg	565.61	J/molxK	672.85	Joback Method
cpg	584.99	J/molxK	708.34	Joback Method
cpg	603.18	J/molxK	743.83	Joback Method
cpg	620.22	J/molxK	779.32	Joback Method
dvisc	0.0023414	Paxs	288.73	Joback Method
dvisc	0.0014305	Paxs	335.00	Joback Method

dvisc	0.0009850	Paxs	381.28	Joback Method
dvisc	0.0007353	Paxs	427.55	Joback Method
dvisc	0.0005812	Paxs	473.82	Joback Method
dvisc	0.0004790	Paxs	520.10	Joback Method
dvisc	0.0004074	Paxs	566.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R413353&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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