

«delta»-Cebebene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24/c1-9(2)12-6-5-11(4)15-8-7-10(3)13(15)14(12)15/h7-14H,5-6H2,1-4H3

DFBLVEBCAFIEDH-PCQKMURISA-N

C15H24

CC(C)C1CCC(C)C23C=CC(C)C2C13

204.35

Physical Properties

Property code	Value	Unit	Source
gf	244.47	kJ/mol	Joback Method
hf	-133.97	kJ/mol	Joback Method
hfus	21.53	kJ/mol	Joback Method
hvap	46.72	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	4.127		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1349.00		NIST Webbook
tb	552.04	K	Joback Method
tc	764.72	K	Joback Method
tf	306.05	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.73	J/mol×K	552.04	Joback Method
cpg	526.15	J/mol×K	587.49	Joback Method
cpg	548.02	J/mol×K	622.93	Joback Method
cpg	568.53	J/mol×K	658.38	Joback Method
cpg	587.84	J/mol×K	693.83	Joback Method
cpg	606.13	J/mol×K	729.28	Joback Method
cpg	623.58	J/mol×K	764.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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