albene

Inchi: InChI=1S/C12H18/c1-11-6-3-7-12(11,2)10-5-4-9(11)8-10/h3,6,9-10H,4-5,7-8H2,1-2H3
InchiKey: HKLBEHRJWPWLOB-UHFFFAOYSA-N
Formula: C12H18
SMILES: CC12C=CCC1(C)C1CCC2C1
Mol. weight [g/mol]: 162.27
CAS: 38451-64-8

Physical Properties

Property code	Value	Unit	Source
gf	231.58	kJ/mol	Joback Method
hf	-10.85	kJ/mol	Joback Method
hfus	8.84	kJ/mol	Joback Method
hvap	39.90	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.389		Crippen Method
mcvol	143.060	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	1161.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1166.90		NIST Webbook
rinpol	1166.90		NIST Webbook
tb	493.42	K	Joback Method
tc	721.89	K	Joback Method
tf	319.62	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.54	J/mol×K	493.42	Joback Method
cpg	372.79	J/mol×K	531.50	Joback Method
cpg	392.03	J/mol×K	569.58	Joback Method
cpg	409.59	J/mol×K	607.66	Joback Method
cpg	425.79	J/mol×K	645.74	Joback Method

cpg	440.95	J/mol×K	683.81	Joback Method
cpg	455.40	J/mol×K	721.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38451648&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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