

Bicyclo[2.2.1]heptan-1-ol

Inchi:	InChI=1S/C7H12O/c8-7-3-1-6(5-7)2-4-7/h6,8H,1-5H2
InchiKey:	NIZFPIBTGJOVRT-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	OC12CCC(CC1)C2
Mol. weight [g/mol]:	112.17

Physical Properties

Property code	Value	Unit	Source
gf	-24.85	kJ/mol	Joback Method
hf	-185.36	kJ/mol	Joback Method
hfus	5.85	kJ/mol	Joback Method
hvap	46.70	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.311		Crippen Method
mcvol	93.640	ml/mol	McGowan Method
pc	4640.32	kPa	Joback Method
rinpol	942.00		NIST Webbook
rinpol	942.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1495.00		NIST Webbook
tb	469.73	K	Joback Method
tc	671.19	K	Joback Method
tf	285.73	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.65	J/mol×K	469.73	Joback Method
cpg	231.01	J/mol×K	503.31	Joback Method
cpg	243.28	J/mol×K	536.88	Joback Method
cpg	254.58	J/mol×K	570.46	Joback Method
cpg	265.03	J/mol×K	604.04	Joback Method
cpg	274.77	J/mol×K	637.62	Joback Method

Sources

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=R13030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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