Benzene, [(cyclohex-1-en-1-yl)methyl]-

Other names: (1-cyclohexen-1-ylmethyl)benzene
Inchi: InChI=1S/C13H16/c1-3-7-12(8-4-1)11-13-9-5-2-6-10-13/h1,3-4,7-9H,2,5-6,10-11H2
InchiKey: CXMRFPAKDYKJJZ-UHFFFAOYSA-N
Formula: C13H16
SMILES: C1=C(Cc2ccccc2)CCCC1
Mol. weight [g/mol]: 172.27
CAS: 4714-09-4

Physical Properties

Property code	Value	Unit	Source
gf	223.48	kJ/mol	Joback Method
hf	45.85	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	48.50	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.729		Crippen Method
mcvol	155.110	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	551.88	K	Joback Method
tc	791.53	K	Joback Method
tf	287.59	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.48	J/mol×K	551.88	Joback Method
cpg	447.70	J/mol×K	751.59	Joback Method
cpg	433.18	J/mol×K	711.65	Joback Method
cpg	417.47	J/mol×K	671.71	Joback Method
cpg	400.50	J/mol×K	631.76	Joback Method
cpg	382.19	J/mol×K	591.82	Joback Method
cpg	461.09	J/mol×K	791.53	Joback Method
dvisc	0.0001872	Pa×s	551.88	Joback Method

dvisc	0.0002482	Pa×s	507.83	Joback Method
dvisc	0.0003470	Pa×s	463.78	Joback Method
dvisc	0.0005206	Pa×s	419.74	Joback Method
dvisc	0.0008591	Pa×s	375.69	Joback Method
dvisc	0.0016192	Pa×s	331.64	Joback Method
dvisc	0.0037061	Pa×s	287.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4714094&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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