

Bicyclo(2.2.1)heptane-2-carboxylic acid

Other names:	2-Norbornanecarboxylic acid endo-Bicyclo(2.2.1)heptane-2-carboxylic acid Bicyclo(2,2,1)heptane-2-carboxylic acid
Inchi:	InChI=1S/C8H12O2/c9-8(10)7-4-5-1-2-6(7)3-5/h5-7H,1-4H2,(H,9,10)
InchiKey:	JESWDXIHOJGWBP-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	O=C(O)C1CC2CCC1C2
Mol. weight [g/mol]:	140.18
CAS:	824-62-4

Physical Properties

Property code	Value	Unit	Source
gf	-147.57	kJ/mol	Joback Method
hf	-354.16	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.507		Crippen Method
mcvol	109.300	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	541.57	K	Joback Method
tc	741.38	K	Joback Method
tf	318.79	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.77	J/molxK	541.57	Joback Method
cpg	339.89	J/molxK	708.08	Joback Method
cpg	329.72	J/molxK	674.78	Joback Method
cpg	318.88	J/molxK	641.48	Joback Method
cpg	307.30	J/molxK	608.17	Joback Method
cpg	294.95	J/molxK	574.87	Joback Method

cpg	349.43	J/molxK	741.38	Joback Method
dvisc	0.0005645	Paxs	541.57	Joback Method
dvisc	0.0007372	Paxs	504.44	Joback Method
dvisc	0.0010044	Paxs	467.31	Joback Method
dvisc	0.0014435	Paxs	430.18	Joback Method
dvisc	0.0022216	Paxs	393.05	Joback Method
dvisc	0.0037411	Paxs	355.92	Joback Method
dvisc	0.0071130	Paxs	318.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.50 ± 0.50	K	2.10	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C824624&Units=SI

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

tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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