Exo-bicyclo(2.2.1)hept-5-ene-2-carboxylic acid

Inchi: InChI=1S/C8H10O2/c9-8(10)7-4-5-1-2-6(7)3-5/h1-2,5-7H,3-4H2,(H,9,10)/t5?,6-,7-/m0/s1
InchiKey: FYGUSUBEMUKACF-BYRXKDITSA-N
Formula: C8H10O2
SMILES: O=C(O)C1CC2C=CC1C2
Mol. weight [g/mol]: 138.16
CAS: 934-30-5

Physical Properties

Property code	Value	Unit	Source
gf	-117.61	kJ/mol	Joback Method
hf	-296.38	kJ/mol	Joback Method
hfus	18.63	kJ/mol	Joback Method
hvap	56.81	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.283		Crippen Method
mcvol	105.000	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
tb	540.73	K	Joback Method
tc	742.39	K	Joback Method
tf	319.55	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.31	J/mol×K	540.73	Joback Method
cpg	275.36	J/mol×K	574.34	Joback Method
cpg	286.60	J/mol×K	607.95	Joback Method
cpg	297.10	J/mol×K	641.56	Joback Method
cpg	306.91	J/mol×K	675.17	Joback Method
cpg	316.07	J/mol×K	708.78	Joback Method
cpg	324.64	J/mol×K	742.39	Joback Method
dvisc	0.0062035	Pa×s	319.55	Joback Method
dvisc	0.0033892	Pa×s	356.41	Joback Method

dvisc	0.0020738	Pa×s	393.28	Joback Method
dvisc	0.0013804	Pa×s	430.14	Joback Method
dvisc	0.0009798	Pa×s	467.00	Joback Method
dvisc	0.0007313	Pa×s	503.87	Joback Method
dvisc	0.0005680	Pa×s	540.73	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.60	K	2.90	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C934305&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
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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