Bicyclo[2.2.1]heptan-1-carboxylic acid, methyl ester

Other names: Methyl bicyclo(2.2.1)heptane-1-carboxylate
Inchi: InChI=1S/C9H14O2/c1-11-8(10)9-4-2-7(6-9)3-5-9/h7H,2-6H2,1H3
InchiKey: ICBCULSDMSBNNZ-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: COC(=O)C12CCC(CC1)C2
Mol. weight [g/mol]: 154.21
CAS: 2287-57-2

Physical Properties

Property code	Value	Unit	Source
gf	-105.11	kJ/mol	Joback Method
hf	-319.21	kJ/mol	Joback Method
hfus	9.72	kJ/mol	Joback Method
hvap	43.63	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.740		Crippen Method
mcvol	123.390	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	1120.00		NIST Webbook
rinpol	1092.00		NIST Webbook
ripol	1487.00		NIST Webbook
tb	499.60	K	Joback Method
tc	717.55	K	Joback Method
tf	319.61	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.31	J/mol×K	499.60	Joback Method
cpg	310.50	J/mol×K	535.92	Joback Method
cpg	325.46	J/mol×K	572.25	Joback Method
cpg	339.35	J/mol×K	608.57	Joback Method
cpg	352.32	J/mol×K	644.90	Joback Method

cpg	364.49	J/mol×K	681.22	Joback Method
cpg	376.03	J/mol×K	717.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	325.50 ± 0.50	K	0.24	NIST Webbook

Sources

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=C2287572&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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