2,3-Dimethyltricyclo[2.2.1.02,6]heptane-3-carboxylic acid

Inchi: InChI=1S/C10H14O2/c1-9(8(11)12)5-3-6-7(4-5)10(6,9)2/h5-7H,3-4H2,1-2H3,(H,11,12)
InchiKey: QHDPITNBVDSMQH-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC1(C(=O)O)C2CC3C(C2)C31C
Mol. weight [g/mol]: 166.22
CAS: 562-66-3

Physical Properties

Property code	Value	Unit	Source
gf	-52.37	kJ/mol	Joback Method
hf	-294.02	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.753		Crippen Method
mcvol	126.620	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1271.20		NIST Webbook
tb	577.07	K	Joback Method
tc	779.86	K	Joback Method
tf	413.39	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.84	J/mol×K	577.07	Joback Method
cpg	370.23	J/mol×K	610.87	Joback Method
cpg	381.73	J/mol×K	644.67	Joback Method
cpg	392.55	J/mol×K	678.46	Joback Method
cpg	402.92	J/mol×K	712.26	Joback Method
cpg	413.10	J/mol×K	746.06	Joback Method
cpg	423.30	J/mol×K	779.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C562663&Units=SI

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

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