6,6-dimethylbicyclo[3.1.1]hept-2-ene-2-carboxylic acid

Other names: Myrtenoic acid
Inchi: InChI=1S/C10H14O2/c1-10(2)6-3-4-7(9(11)12)8(10)5-6/h4,6,8H,3,5H2,1-2H3,(H,11,12)
InchiKey: XPHVDOXZJRTIMV-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC1(C)C2CC=C(C(=O)O)C1C2
Mol. weight [g/mol]: 166.22
CAS: 19250-17-0

Physical Properties

Property code	Value	Unit	Source
gf	-115.89	kJ/mol	Joback Method
hf	-333.89	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	60.77	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.063		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1359.00		NIST Webbook
tb	591.71	K	Joback Method
tc	796.05	K	Joback Method
tf	378.51	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.13	J/mol×K	591.71	Joback Method
cpg	366.94	J/mol×K	625.77	Joback Method
cpg	378.97	J/mol×K	659.82	Joback Method
cpg	390.35	J/mol×K	693.88	Joback Method
cpg	401.20	J/mol×K	727.93	Joback Method
cpg	411.64	J/mol×K	761.99	Joback Method
cpg	421.81	J/mol×K	796.05	Joback Method

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=C19250170&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume