(E)-5-((1R,3R,6S)-2,3-Dimethyltricyclo[2.2.1.02,6]h
acid

Inchi: InChI=1S/C15H22O2/c1-9(13(16)17)5-4-6-14(2)10-7-11-12(8-10)15(11,14)3/h5,10-12H,4

InchiKey: NZSCHTYUGUVLHG-WEVVVXLNSA-N

Formula: C15H22O2

SMILES: CC(=CCCC1(C)C2CC3C(C2)C31C)C(=O)O

Mol. weight [g/mol]: 234.33

CAS: 74642-79-8

Physical Properties

Property code	Value	Unit	Source
gf	61.40	kJ/mol	Joback Method
hf	-289.79	kJ/mol	Joback Method
hfus	27.34	kJ/mol	Joback Method
hvap	68.92	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.480		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1847.40		NIST Webbook
rinpol	1847.40		NIST Webbook
tb	695.51	K	Joback Method
tc	895.67	K	Joback Method
tf	450.70	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.97	J/mol×K	695.51	Joback Method
cpg	602.10	J/mol×K	728.87	Joback Method
cpg	616.87	J/mol×K	762.23	Joback Method
cpg	631.53	J/mol×K	795.59	Joback Method
cpg	646.33	J/mol×K	828.95	Joback Method
cpg	661.52	J/mol×K	862.31	Joback Method
cpg	677.34	J/mol×K	895.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74642798&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
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