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

Inchi: InChI=1S/C15H22O/c1-10(9-16)5-4-6-14(2)11-7-12-13(8-11)15(12,14)3/h5,9,11-13H,4,6-
InchiKey: SHEUEEZGXLCROM-BJMVGYQFSA-N
Formula: C15H22O
SMILES: CC(C=O)=CCCC1(C)C2CC3C(C2)C31C
Mol. weight [g/mol]: 218.33
CAS: 19903-70-9

Physical Properties

Property code	Value	Unit	Source
gf	227.62	kJ/mol	Joback Method
hf	-110.56	kJ/mol	Joback Method
hfus	23.94	kJ/mol	Joback Method
hvap	52.22	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1679.30		NIST Webbook
rinpol	1679.30		NIST Webbook
ripol	2196.00		NIST Webbook
ripol	2196.00		NIST Webbook
tb	598.12	K	Joback Method
tc	806.92	K	Joback Method
tf	381.95	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.42	J/mol×K	598.12	Joback Method
cpg	542.34	J/mol×K	632.92	Joback Method
cpg	559.12	J/mol×K	667.72	Joback Method
cpg	575.05	J/mol×K	702.52	Joback Method
cpg	590.41	J/mol×K	737.32	Joback Method

cpg	605.48	J/mol×K	772.12	Joback Method
cpg	620.53	J/mol×K	806.92	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=C19903709&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume