5-(2,3-Dimethyltricyclo[2.2.1.02,6]heptan-3-yl)pent

Inchi: InChI=1S/C14H22O/c1-9(15)5-4-6-13(2)10-7-11-12(8-10)14(11,13)3/h10-12H,4-8H2,1-3
InchiKey: IBSHUAUUJQYONI-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CC(=O)CCCC1(C)C2CC3C(C2)C31C
Mol. weight [g/mol]: 206.32
CAS: 60843-83-6

Physical Properties

Property code	Value	Unit	Source
gf	118.13	kJ/mol	Joback Method
hf	-224.35	kJ/mol	Joback Method
hfus	21.77	kJ/mol	Joback Method
hvap	49.98	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.428		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1522.50		NIST Webbook
rinpol	1522.50		NIST Webbook
tb	576.41	K	Joback Method
tc	780.91	K	Joback Method
tf	397.65	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.15	J/mol×K	576.41	Joback Method
cpg	511.25	J/mol×K	610.49	Joback Method
cpg	528.15	J/mol×K	644.58	Joback Method
cpg	544.10	J/mol×K	678.66	Joback Method
cpg	559.36	J/mol×K	712.74	Joback Method
cpg	574.15	J/mol×K	746.83	Joback Method
cpg	588.74	J/mol×K	780.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60843836&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