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

Inchi: InChI=1S/C12H18O/c1-11(4-3-5-13)8-6-9-10(7-8)12(9,11)2/h5,8-10H,3-4,6-7H2,1-2H3
InchiKey: GBXFUOBZYUTFOP-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC1(CCC=O)C2CC3C(C2)C31C
Mol. weight [g/mol]: 178.27
CAS: 16933-18-9

Physical Properties

Property code	Value	Unit	Source
gf	130.69	kJ/mol	Joback Method
hf	-156.07	kJ/mol	Joback Method
hfus	17.28	kJ/mol	Joback Method
hvap	45.50	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.648		Crippen Method
mcvol	148.930	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1343.00		NIST Webbook
tb	525.44	K	Joback Method
tc	731.34	K	Joback Method
tf	367.18	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.00	J/mol×K	525.44	Joback Method
cpg	412.16	J/mol×K	559.76	Joback Method
cpg	427.89	J/mol×K	594.07	Joback Method
cpg	442.44	J/mol×K	628.39	Joback Method
cpg	456.07	J/mol×K	662.71	Joback Method
cpg	469.01	J/mol×K	697.02	Joback Method
cpg	481.53	J/mol×K	731.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16933189&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