(2S*,5R*)-2-formylmethyl-2-methyl-5-(1-hydroxy-1

Inchi: InChI=1S/C10H18O3/c1-9(2,12)8-4-5-10(3,13-8)6-7-11/h7-8,12H,4-6H2,1-3H3/t8-,10+/m
InchiKey: WRGPONPRWKAHCK-WCBMZHEXSA-N
Formula: C10H18O3
SMILES: CC1(CC=O)CCC(C(C)(C)O)O1
Mol. weight [g/mol]: 186.25

Physical Properties

Property code	Value	Unit	Source
gf	-262.95	kJ/mol	Joback Method
hf	-572.91	kJ/mol	Joback Method
hfus	17.31	kJ/mol	Joback Method
hvap	63.26	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.284		Crippen Method
mcvol	154.210	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1254.00		NIST Webbook
tb	603.61	K	Joback Method
tc	803.67	K	Joback Method
tf	364.83	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.96	J/mol×K	603.61	Joback Method
cpg	439.14	J/mol×K	636.95	Joback Method
cpg	452.49	J/mol×K	670.30	Joback Method
cpg	465.13	J/mol×K	703.64	Joback Method
cpg	477.14	J/mol×K	736.98	Joback Method
cpg	488.65	J/mol×K	770.33	Joback Method
cpg	499.77	J/mol×K	803.67	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=R342751&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