6-Hydroxycarvotanacetone

Inchi: InChI=1S/C10H16O2/c1-6(2)8-5-4-7(3)9(11)10(8)12/h4,6,8,10,12H,5H2,1-3H3
InchiKey: CSTXLFNLXWTVDQ-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC1=CCC(C(C)C)C(O)C1=O
Mol. weight [g/mol]: 168.24

Physical Properties

Property code	Value	Unit	Source
hfus	15.47	kJ/mol	Joback Method
logp	1.539		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
rinpol	1317.80		NIST Webbook
rinpol	1317.80		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.06	J/mol×K	606.78	Joback Method
cpg	398.33	J/mol×K	641.05	Joback Method
cpg	412.83	J/mol×K	675.32	Joback Method
cpg	426.57	J/mol×K	709.59	Joback Method
cpg	439.53	J/mol×K	743.86	Joback Method
cpg	451.71	J/mol×K	778.13	Joback Method
cpg	463.09	J/mol×K	812.40	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C131486992&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices