Benzoyl(cyclohexyloxy)-carbonylperoxide

Inchi: InChI=1S/C14H16O5/c15-13(11-7-3-1-4-8-11)18-19-14(16)17-12-9-5-2-6-10-12/h1,3-4,7-
InchiKey: XHRPWCKLJGNVSL-UHFFFAOYSA-N
Formula: C14H16O5
SMILES: O=C(OOC(=O)c1ccccc1)OC1CCCCC1
Mol. weight [g/mol]: 264.27
CAS: 20666-86-8

Physical Properties

Property code	Value	Unit	Source
chs	-7054.20 ± 8.40	kJ/mol	NIST Webbook
gf	-368.98	kJ/mol	Joback Method
hf	-645.30 ± 9.40	kJ/mol	NIST Webbook
hfs	-741.50 ± 8.40	kJ/mol	NIST Webbook
hfus	24.65	kJ/mol	Joback Method
hsub	96.20	kJ/mol	NIST Webbook
hvap	70.19	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.244		Crippen Method
mcvol	194.250	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
tb	740.95	K	Joback Method
tc	975.09	K	Joback Method
tf	447.89	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.14	J/mol×K	740.95	Joback Method
cpg	576.37	J/mol×K	779.97	Joback Method
cpg	591.19	J/mol×K	819.00	Joback Method
cpg	604.62	J/mol×K	858.02	Joback Method
cpg	616.65	J/mol×K	897.05	Joback Method
cpg	627.28	J/mol×K	936.07	Joback Method

cpg	636.52	J/mol×K	975.09	Joback Method
dvisc	0.0009933	Pa×s	447.89	Joback Method
dvisc	0.0005558	Pa×s	496.73	Joback Method
dvisc	0.0003450	Pa×s	545.58	Joback Method
dvisc	0.0002317	Pa×s	594.42	Joback Method
dvisc	0.0001652	Pa×s	643.26	Joback Method
dvisc	0.0001236	Pa×s	692.11	Joback Method
dvisc	0.0000961	Pa×s	740.95	Joback Method
hsubt	96.20 ± 4.20	kJ/mol	303.00	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20666868&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume