2,2-dimethyl-1-(2-hydroxy-1-methylethyl)propyl-2-

Inchi: InChI=1S/C13H26O3/c1-9(8-14)10(12(2,3)4)16-11(15)13(5,6)7/h9-10,14H,8H2,1-7H3
InchiKey: FEZQUOCHDRVWLJ-UHFFFAOYSA-N
Formula: C13H26O3
SMILES: CC(CO)C(OC(=O)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 230.34

Physical Properties

Property code	Value	Unit	Source
gf	-311.36	kJ/mol	Joback Method
hf	-736.74	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.619		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
ripol	1882.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1882.00		NIST Webbook
tb	657.97	K	Joback Method
tc	842.71	K	Joback Method
tf	344.09	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.53	J/mol×K	657.97	Joback Method
cpg	658.79	J/mol×K	811.92	Joback Method
cpg	646.50	J/mol×K	781.13	Joback Method
cpg	633.47	J/mol×K	750.34	Joback Method
cpg	619.66	J/mol×K	719.55	Joback Method
cpg	605.03	J/mol×K	688.76	Joback Method

cpg	670.38	J/mol×K	842.71	Joback Method
dvisc	0.0000290	Pa×s	657.97	Joback Method
dvisc	0.0000502	Pa×s	605.66	Joback Method
dvisc	0.0000964	Pa×s	553.34	Joback Method
dvisc	0.0002121	Pa×s	501.03	Joback Method
dvisc	0.0005609	Pa×s	448.72	Joback Method
dvisc	0.0019173	Pa×s	396.40	Joback Method
dvisc	0.0095233	Pa×s	344.09	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=R495855&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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