4-hydroxybutyl hexanoate

Inchi: InChI=1S/C10H20O3/c1-2-3-4-7-10(12)13-9-6-5-8-11/h11H,2-9H2,1H3
InchiKey: CXCIGAYDAQVVRU-UHFFFAOYSA-N
Formula: C10H20O3
SMILES: CCCCCC(=O)OCCCCO
Mol. weight [g/mol]: 188.26

Physical Properties

Property code	Value	Unit	Source
gf	-337.42	kJ/mol	Joback Method
hf	-646.76	kJ/mol	Joback Method
hfus	28.53	kJ/mol	Joback Method
hvap	63.69	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.882		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
ripol	1666.00		NIST Webbook
tb	596.67	K	Joback Method
tc	763.64	K	Joback Method
tf	335.44	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.51	J/mol×K	596.67	Joback Method
cpg	440.83	J/mol×K	624.50	Joback Method
cpg	452.65	J/mol×K	652.33	Joback Method
cpg	463.99	J/mol×K	680.16	Joback Method
cpg	474.85	J/mol×K	707.98	Joback Method
cpg	485.23	J/mol×K	735.81	Joback Method
cpg	495.14	J/mol×K	763.64	Joback Method
dvisc	0.0060280	Pa×s	335.44	Joback Method
dvisc	0.0019204	Pa×s	378.98	Joback Method

dvisc	0.0007745	Pa×s	422.52	Joback Method
dvisc	0.0003701	Pa×s	466.05	Joback Method
dvisc	0.0002006	Pa×s	509.59	Joback Method
dvisc	0.0001198	Pa×s	553.13	Joback Method
dvisc	0.0000771	Pa×s	596.67	Joback Method

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=R519109&Units=SI

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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