

2-(2'-Hydroxyethoxy)ethyl pivalate

Inchi:	InChI=1S/C9H18O4/c1-9(2,3)8(11)13-7-6-12-5-4-10/h10H,4-7H2,1-3H3
InchiKey:	OIJDLOHUGUWXRT-UHFFFAOYSA-N
Formula:	C9H18O4
SMILES:	CC(C)(C)C(=O)OCCOCCO
Mol. weight [g/mol]:	190.24
CAS:	20267-21-4

Physical Properties

Property code	Value	Unit	Source
gf	-448.00	kJ/mol	Joback Method
hf	-767.09	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	62.58	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	0.585		Crippen Method
mvol	156.850	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
tb	592.98	K	Joback Method
tc	768.33	K	Joback Method
tf	348.82	K	Joback Method
vc	0.590	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.41	J/molxK	768.33	Joback Method
cpg	463.04	J/molxK	739.11	Joback Method
cpg	453.17	J/molxK	709.88	Joback Method
cpg	442.78	J/molxK	680.66	Joback Method
cpg	431.86	J/molxK	651.43	Joback Method
cpg	420.41	J/molxK	622.21	Joback Method
cpg	408.42	J/molxK	592.98	Joback Method
cpl	311.60	J/molxK	298.15	NIST Webbook
dvisc	0.0000966	Paxs	552.29	Joback Method

dvisc	0.0001624	Paxs	511.59	Joback Method
dvisc	0.0002987	Paxs	470.90	Joback Method
dvisc	0.0006167	Paxs	430.21	Joback Method
dvisc	0.0014812	Paxs	389.51	Joback Method
dvisc	0.0043648	Paxs	348.82	Joback Method
dvisc	0.0000617	Paxs	592.98	Joback Method

Sources

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=C20267214&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
cp_l:	Liquid phase 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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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