2-Hydroxyethyl heptanoate

Inchi: InChI=1S/C9H18O3/c1-2-3-4-5-6-9(11)12-8-7-10/h10H,2-8H2,1H3
InchiKey: OPIZFHYNWKYUKL-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: CCCCCCC(=O)OCCO
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
gf	-345.84	kJ/mol	Joback Method
hf	-626.12	kJ/mol	Joback Method
hfus	25.94	kJ/mol	Joback Method
hvap	61.46	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.492		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1294.00		NIST Webbook
tb	573.79	K	Joback Method
tc	741.45	K	Joback Method
tf	324.17	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.06	J/mol×K	573.79	Joback Method
cpg	391.64	J/mol×K	601.73	Joback Method
cpg	402.75	J/mol×K	629.68	Joback Method
cpg	413.43	J/mol×K	657.62	Joback Method
cpg	423.65	J/mol×K	685.56	Joback Method
cpg	433.44	J/mol×K	713.51	Joback Method
cpg	442.80	J/mol×K	741.45	Joback Method
dvisc	0.0071971	Pa×s	324.17	Joback Method
dvisc	0.0023045	Pa×s	365.77	Joback Method

dvisc	0.0009311	Pa×s	407.38	Joback Method
dvisc	0.0004450	Pa×s	448.98	Joback Method
dvisc	0.0002411	Pa×s	490.58	Joback Method
dvisc	0.0001437	Pa×s	532.19	Joback Method
dvisc	0.0000924	Pa×s	573.79	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=R540495&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume