

2-Hydroxyethyl caprylate

Inchi:	InChI=1S/C10H20O3/c1-2-3-4-5-6-7-10(12)13-9-8-11/h11H,2-9H2,1H3
InchiKey:	CBLFQQQLPYAQCP-UHFFFAOYSA-N
Formula:	C10H20O3
SMILES:	CCCCCCCC(=O)OCCO
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
rinsol	1396.00		NIST Webbook
tb	596.67	K	Joback Method
tc	763.64	K	Joback Method
tf	335.44	K	Joback Method
vc	0.638	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.51	J/molxK	596.67	Joback Method
cpg	485.23	J/molxK	735.81	Joback Method
cpg	474.85	J/molxK	707.98	Joback Method
cpg	463.99	J/molxK	680.16	Joback Method
cpg	452.65	J/molxK	652.33	Joback Method
cpg	440.83	J/molxK	624.50	Joback Method
cpg	495.14	J/molxK	763.64	Joback Method
dvisc	0.0000771	Paxs	596.67	Joback Method
dvisc	0.0001198	Paxs	553.13	Joback Method

dvisc	0.0002006	Paxs	509.59	Joback Method
dvisc	0.0003701	Paxs	466.05	Joback Method
dvisc	0.0007745	Paxs	422.52	Joback Method
dvisc	0.0019204	Paxs	378.98	Joback Method
dvisc	0.0060280	Paxs	335.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540475&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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