2-HYDROXYHEXADECYL BUTANOATE

Inchi: InChI=1S/C20H40O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-17-19(21)18-23-20(22)16-4-2/h1
InchiKey: IOSQACMVRMGUJE-UHFFFAOYSA-N
Formula: C20H40O3
SMILES: CCCCCCCCCCCCCCC(O)COC(=O)CCC
Mol. weight [g/mol]: 328.54

Physical Properties

Property code	Value	Unit	Source
af	1.1189		Cheméo Relay (1.0)
hf	-947.97	kJ/mol	Cheméo Relay (1.0)
hfus	50.91	kJ/mol	Joback Method
hvap	117.68	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.55		Cheméo Relay (1.0)
logp	5.782		Crippen Method
mcvol	305.970	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
tb	616.50	K	Cheméo Relay (1.0)
tc	804.02	K	Cheméo Relay (1.0)
tf	317.40	K	Cheméo Relay (1.0)
vc	1.188	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.35	J/mol×K	825.03	Joback Method
cpg	1005.56	J/mol×K	855.88	Joback Method
cpg	1022.77	J/mol×K	886.73	Joback Method
cpg	1039.01	J/mol×K	917.58	Joback Method
cpg	1054.31	J/mol×K	948.42	Joback Method
cpg	1068.70	J/mol×K	979.27	Joback Method
cpg	1082.21	J/mol×K	1010.12	Joback Method
dvisc	0.0012770	Pa×s	433.14	Joback Method
dvisc	0.0003457	Pa×s	498.45	Joback Method
dvisc	0.0001267	Pa×s	563.77	Joback Method

dvisc	0.0000572	Pa×s	629.09	Joback Method
dvisc	0.0000300	Pa×s	694.40	Joback Method
dvisc	0.0000176	Pa×s	759.71	Joback Method
dvisc	0.0000112	Pa×s	825.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77899015&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume