Pimelic acid, 2-ethylbutyl hexyl ester

Inchi: InChI=1S/C19H36O4/c1-4-7-8-12-15-22-18(20)13-10-9-11-14-19(21)23-16-17(5-2)6-3/h1
InchiKey: UYNNAEUNFOISBN-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CCCCCCOC(=O)CCCCCC(=O)OCC(CC)CC
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-361.18	kJ/mol	Joback Method
hf	-930.37	kJ/mol	Joback Method
hfus	47.02	kJ/mol	Joback Method
hvap	75.81	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	5.040		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1155.35	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
tb	786.26	K	Joback Method
tc	968.16	K	Joback Method
tf	433.21	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.39	J/mol×K	786.26	Joback Method
cpg	989.26	J/mol×K	937.85	Joback Method
cpg	975.21	J/mol×K	907.53	Joback Method
cpg	960.22	J/mol×K	877.21	Joback Method
cpg	944.26	J/mol×K	846.89	Joback Method
cpg	927.32	J/mol×K	816.58	Joback Method
cpg	1002.36	J/mol×K	968.16	Joback Method
dvisc	0.0000565	Pa×s	786.26	Joback Method

dvisc	0.0000759	Pa×s	727.42	Joback Method
dvisc	0.0001075	Pa×s	668.58	Joback Method
dvisc	0.0001628	Pa×s	609.74	Joback Method
dvisc	0.0002693	Pa×s	550.89	Joback Method
dvisc	0.0005025	Pa×s	492.05	Joback Method
dvisc	0.0011109	Pa×s	433.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406631&Units=SI
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

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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