Triethylene glycol di(2-ethylhexoate)

Other names:	Hexanoic acid, 2-ethyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester
	Hexanoic acid, 2-ethyl-, diester with triethylene glycol
	Flexol plasticizer 3GO
	Triethylene glycol, bis(ethylhexanoate)
	Kodaflex TEG-EH
	Ethane, 1,2-(2'-hydroxyethoxy)-, di-(2-ethylhexanoate)-
	Triethylene glycol, bis[2-ethylhexyl] ester
	Hexanoic acid, 2-ethyl-, 1,1'-[1,2-ethanediylbis(oxy-2,1-ethanediyl)] ester
	Triethylene glycol, bis(2-ethylhexanoate)
	Triethylene glycol, bis[2-ethylhexyl] etser
	2,2'-ethylenedioxydiethyl bis(2-ethylhexanoate)
Inchi:	InChI=1S/C22H42O6/c1-5-9-11-19(7-3)21(23)27-17-15-25-13-14-26-16-18-28-22(24)20(
InchiKey:	FRQDZJMEHSJOPU-UHFFFAOYSA-N
Formula:	C22H42O6
SMILES:	CCCCC(CC)C(=O)OCCOCCOCCOC(=O)C(CC)CCCC
Mol. weight [g/mol]:	402.57
CAS:	94-28-0

Physical Properties

Property code	Value	Unit	Source
gf	-548.36	kJ/mol	Joback Method
hf	-1262.01	kJ/mol	Joback Method
hfus	53.64	kJ/mol	Joback Method
hvap	86.92	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.539		Crippen Method
mcvol	347.460	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
tb	899.30	K	Joback Method
tc	1101.28	K	Joback Method
tf	496.48	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.64	J/mol×K	899.30	Joback Method
cpg	1234.03	J/mol×K	1067.62	Joback Method
cpg	1221.55	J/mol×K	1033.95	Joback Method
cpg	1207.57	J/mol×K	1000.29	Joback Method
cpg	1192.09	J/mol×K	966.63	Joback Method
cpg	1175.12	J/mol×K	932.96	Joback Method
cpg	1245.02	J/mol×K	1101.28	Joback Method
dvisc	0.0000182	Pa×s	899.30	Joback Method
dvisc	0.0000248	Pa×s	832.16	Joback Method
dvisc	0.0000357	Pa×s	765.03	Joback Method
dvisc	0.0000549	Pa×s	697.89	Joback Method
dvisc	0.0000928	Pa×s	630.75	Joback Method
dvisc	0.0001777	Pa×s	563.62	Joback Method
dvisc	0.0004054	Pa×s	496.48	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94280&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume