

TRIETHYLENEGLYCOL DI-2-ETHYLHEXAOATE

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

Physical Properties

Property code	Value	Unit	Source
hf	-1361.41	kJ/mol	Cheméo Relay (1.0)
hfus	53.64	kJ/mol	Joback Method
hvap	105.33	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.38		Cheméo Relay (1.0)
logp	4.539		Crippen Method
mcvol	347.460	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
tb	630.05	K	Cheméo Relay (1.0)
tc	809.45	K	Cheméo Relay (1.0)
tf	219.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.64	J/mol×K	899.30	Joback Method

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

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C94280&Units=SI

Legend

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

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