

Triethylene glycol dioctanoate

Other names:	2,2'-ethylenedioxydiethyl dioctanoate
Inchi:	InChI=1S/C22H42O6/c1-3-5-7-9-11-13-21(23)27-19-17-25-15-16-26-18-20-28-22(24)14-
InchiKey:	YJGHMLJGPSVSLF-UHFFFAOYSA-N
Formula:	C22H42O6
SMILES:	CCCCCCCC(=O)OCCOCCOCCOC(=O)CCCCCCC
Mol. weight [g/mol]:	402.57
CAS:	106-10-5

Physical Properties

Property code	Value	Unit	Source
gf	-543.48	kJ/mol	Joback Method
hf	-1251.45	kJ/mol	Joback Method
hfus	60.69	kJ/mol	Joback Method
hvap	87.70	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.827		Crippen Method
mcvol	347.460	ml/mol	McGowan Method
pc	934.06	kPa	Joback Method
tb	900.18	K	Joback Method
tc	1103.22	K	Joback Method
tf	526.48	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.76	J/molxK	900.18	Joback Method
cpg	1233.89	J/molxK	1069.38	Joback Method
cpg	1221.25	J/molxK	1035.54	Joback Method
cpg	1207.12	J/molxK	1001.70	Joback Method
cpg	1191.49	J/molxK	967.86	Joback Method
cpg	1174.38	J/molxK	934.02	Joback Method
cpg	1245.04	J/molxK	1103.22	Joback Method
dvisc	0.0000218	Paxs	900.18	Joback Method

dvisc	0.0000288	Paxs	837.90	Joback Method
dvisc	0.0000398	Paxs	775.61	Joback Method
dvisc	0.0000581	Paxs	713.33	Joback Method
dvisc	0.0000911	Paxs	651.05	Joback Method
dvisc	0.0001574	Paxs	588.76	Joback Method
dvisc	0.0003094	Paxs	526.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106105&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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