TRIETHYLENEGLYCOL DIPELARGONATE

Other names: Triethyleneglycol dipelargonate
ethylenebis(oxyethylene) dinonanoate
Inchi: InChI=1S/C24H46O6/c1-3-5-7-9-11-13-15-23(25)29-21-19-27-17-18-28-20-22-30-24(26)16-14-12-10-8-6-4-2
InchiKey: UBQXQCCAPASFJR-UHFFFAOYSA-N
Formula: C24H46O6
SMILES: CCCCCCCCC(=O)OCCOCCOCCOC(=O)CCCCCCCC
Mol. weight [g/mol]: 430.63

Physical Properties

Property code	Value	Unit	Source
af	1.2592		Cheméo Relay (1.0)
hf	-1384.48	kJ/mol	Cheméo Relay (1.0)
hfus	65.87	kJ/mol	Joback Method
hvap	118.86	kJ/mol	Cheméo Relay (1.0)
ie	9.52	eV	Cheméo Relay (1.0)
log10ws	-5.31		Cheméo Relay (1.0)
logp	5.607		Crippen Method
mcvol	375.640	ml/mol	McGowan Method
pc	833.38	kPa	Joback Method
tb	664.02	K	Cheméo Relay (1.0)
tc	825.91	K	Cheméo Relay (1.0)
tf	278.37	K	Cheméo Relay (1.0)
vc	1.449	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.28	J/mol×K	945.94	Joback Method
cpg	1370.94	J/mol×K	1164.48	Joback Method
cpg	1360.51	J/mol×K	1128.05	Joback Method
cpg	1348.29	J/mol×K	1091.63	Joback Method
cpg	1334.27	J/mol×K	1055.21	Joback Method
cpg	1318.43	J/mol×K	1018.79	Joback Method
cpg	1300.77	J/mol×K	982.36	Joback Method

dvisc	0.0000433	Pa×s	747.48	Joback Method
dvisc	0.0000160	Pa×s	945.94	Joback Method
dvisc	0.0000212	Pa×s	879.79	Joback Method
dvisc	0.0000294	Pa×s	813.63	Joback Method
dvisc	0.0002410	Pa×s	549.02	Joback Method
dvisc	0.0000686	Pa×s	681.33	Joback Method
dvisc	0.0001202	Pa×s	615.17	Joback Method

Sources

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=C106069&Units=SI
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

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
ie:	Ionization energy
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