

Diglycolic acid, nonyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C21H40O5/c1-6-7-8-9-10-11-12-13-25-19(22)16-24-17-20(23)26-15-18(2)14-2
InchiKey:	QFRGYUUHAYZAR-UHFFFAOYSA-N
Formula:	C21H40O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	372.54

Physical Properties

Property code	Value	Unit	Source
gf	-446.50	kJ/mol	Joback Method
hf	-1112.62	kJ/mol	Joback Method
hfus	45.97	kJ/mol	Joback Method
hvap	81.38	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.912		Crippen Method
mcvol	327.500	ml/mol	McGowan Method
pc	1019.43	kPa	Joback Method
rinpola	2937.00		NIST Webbook
rinpola	2937.00		NIST Webbook
tb	851.21	K	Joback Method
tc	1043.75	K	Joback Method
tf	480.40	K	Joback Method
vc	1.260	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.19	J/molxK	851.21	Joback Method
cpg	1143.12	J/molxK	1011.66	Joback Method
cpg	1129.44	J/molxK	979.57	Joback Method
cpg	1114.64	J/molxK	947.48	Joback Method
cpg	1098.68	J/molxK	915.39	Joback Method
cpg	1081.54	J/molxK	883.30	Joback Method
cpg	1155.70	J/molxK	1043.75	Joback Method
dvisc	0.0000248	Paxs	851.21	Joback Method

dvisc	0.0000340	Paxs	789.41	Joback Method
dvisc	0.0000491	Paxs	727.61	Joback Method
dvisc	0.0000760	Paxs	665.81	Joback Method
dvisc	0.0001286	Paxs	604.00	Joback Method
dvisc	0.0002455	Paxs	542.20	Joback Method
dvisc	0.0005533	Paxs	480.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382044&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/84-795-7/Diglycolic-acid-nonyl-2-4-4-trimethylpentyl-ester.pdf>

Generated by Cheméo on 2024-04-24 06:17:01.447429897 +0000 UTC m=+16228670.368007210.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.