

Diglycolic acid, decyl 3,7-dimethyloctyl ester

Inchi:	InChI=1S/C24H46O5/c1-5-6-7-8-9-10-11-12-17-28-23(25)19-27-20-24(26)29-18-16-22(4
InchiKey:	ZJYYDBXWSFPAKM-UHFFFAOYSA-N
Formula:	C24H46O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]:	414.62

Physical Properties

Property code	Value	Unit	Source
gf	-426.52	kJ/mol	Joback Method
hf	-1171.07	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	88.96	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	6.083		Crippen Method
mcvol	369.770	ml/mol	McGowan Method
pc	849.49	kPa	Joback Method
rinpola	3348.00		NIST Webbook
rinpola	3348.00		NIST Webbook
tb	922.64	K	Joback Method
tc	1131.32	K	Joback Method
tf	496.79	K	Joback Method
vc	1.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.53	J/molxK	922.64	Joback Method
cpg	1270.20	J/molxK	957.42	Joback Method
cpg	1288.29	J/molxK	992.20	Joback Method
cpg	1304.80	J/molxK	1026.98	Joback Method
cpg	1319.78	J/molxK	1061.76	Joback Method
cpg	1333.23	J/molxK	1096.54	Joback Method
cpg	1345.19	J/molxK	1131.32	Joback Method
dvisc	0.0004693	Paxs	496.79	Joback Method

dvisc	0.0001943	Paxs	567.76	Joback Method
dvisc	0.0000979	Paxs	638.74	Joback Method
dvisc	0.0000565	Paxs	709.71	Joback Method
dvisc	0.0000361	Paxs	780.69	Joback Method
dvisc	0.0000248	Paxs	851.66	Joback Method
dvisc	0.0000181	Paxs	922.64	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382151&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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