

Glutaric acid, nonyl 2-phenoxyethyl ester

Inchi: InChI=1S/C22H34O5/c1-2-3-4-5-6-7-11-17-26-21(23)15-12-16-22(24)27-19-18-25-20-13
InchiKey: TZQSKZVJFKNOST-UHFFFAOYSA-N
Formula: C22H34O5
SMILES: CCCCCCCCCOC(=O)CCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 378.50

Physical Properties

Property code	Value	Unit	Source
gf	-326.07	kJ/mol	Joback Method
hf	-882.70	kJ/mol	Joback Method
hfus	53.54	kJ/mol	Joback Method
hvap	87.56	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.073		Crippen Method
mvol	317.830	ml/mol	McGowan Method
pc	1169.62	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	904.44	K	Joback Method
tc	1109.57	K	Joback Method
tf	530.67	K	Joback Method
vc	1.226	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.65	J/molxK	904.44	Joback Method
cpg	1043.76	J/molxK	938.63	Joback Method
cpg	1058.53	J/molxK	972.82	Joback Method
cpg	1072.00	J/molxK	1007.01	Joback Method
cpg	1084.17	J/molxK	1041.19	Joback Method
cpg	1095.08	J/molxK	1075.38	Joback Method
cpg	1104.75	J/molxK	1109.57	Joback Method
dvisc	0.0003866	Paxs	530.67	Joback Method

dvisc	0.0002022	Paxs	592.96	Joback Method
dvisc	0.0001196	Paxs	655.26	Joback Method
dvisc	0.0000775	Paxs	717.55	Joback Method
dvisc	0.0000538	Paxs	779.85	Joback Method
dvisc	0.0000395	Paxs	842.14	Joback Method
dvisc	0.0000302	Paxs	904.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376921&Units=SI

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

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