

Glutaric acid, 2-methoxyethyl tridecyl ester

Inchi: InChI=1S/C21H40O5/c1-3-4-5-6-7-8-9-10-11-12-13-17-25-20(22)15-14-16-21(23)26-19-1
InchiKey: JWDOYEAASJRECR-UHFFFAOYSA-N
Formula: C21H40O5
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)OCCOC
Mol. weight [g/mol]: 372.54

Physical Properties

Property code	Value	Unit	Source
gf	-446.90	kJ/mol	Joback Method
hf	-1098.59	kJ/mol	Joback Method
hfus	56.91	kJ/mol	Joback Method
hvap	83.06	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.201		Crippen Method
mcvol	327.500	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	2636.00		NIST Webbook
tb	854.88	K	Joback Method
tc	1046.67	K	Joback Method
tf	492.98	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.15	J/mol×K	854.88	Joback Method
cpg	1080.63	J/mol×K	886.84	Joback Method
cpg	1097.88	J/mol×K	918.81	Joback Method
cpg	1113.92	J/mol×K	950.77	Joback Method
cpg	1128.76	J/mol×K	982.74	Joback Method
cpg	1142.41	J/mol×K	1014.70	Joback Method
cpg	1154.88	J/mol×K	1046.67	Joback Method
dvisc	0.0005115	Pa×s	492.98	Joback Method
dvisc	0.0002551	Pa×s	553.30	Joback Method

dvisc	0.0001459	Pa×s	613.61	Joback Method
dvisc	0.0000922	Pa×s	673.93	Joback Method
dvisc	0.0000628	Pa×s	734.25	Joback Method
dvisc	0.0000454	Pa×s	794.56	Joback Method
dvisc	0.0000343	Pa×s	854.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360110&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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