

Glutaric acid, pentadecyl tetrahydrofurfuryl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C25H46O5/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-29-24(26)18-15-19-25(27)30

XNQJFXZUFYOKM-UHFFFAOYSA-N

C25H46O5

CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC1CCCO1

426.63

Physical Properties

Property code	Value	Unit	Source
gf	-357.79	kJ/mol	Joback Method
hf	-1120.45	kJ/mol	Joback Method
hfus	67.99	kJ/mol	Joback Method
hvap	94.32	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.513		Crippen Method
mcvol	373.000	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	3166.00		NIST Webbook
tb	966.21	K	Joback Method
tc	1184.53	K	Joback Method
tf	553.30	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.91	J/mol×K	966.21	Joback Method
cpg	1328.29	J/mol×K	1002.60	Joback Method
cpg	1346.01	J/mol×K	1038.98	Joback Method
cpg	1362.15	J/mol×K	1075.37	Joback Method
cpg	1376.76	J/mol×K	1111.76	Joback Method
cpg	1389.89	J/mol×K	1148.14	Joback Method
cpg	1401.59	J/mol×K	1184.53	Joback Method
dvisc	0.0004909	Pa×s	553.30	Joback Method
dvisc	0.0002419	Pa×s	622.12	Joback Method

dvisc	0.0001373	Pa×s	690.94	Joback Method
dvisc	0.0000863	Pa×s	759.75	Joback Method
dvisc	0.0000586	Pa×s	828.57	Joback Method
dvisc	0.0000423	Pa×s	897.39	Joback Method
dvisc	0.0000319	Pa×s	966.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359671&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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