

Glutaric acid, 2-biphenyl dodecyl ester

Inchi: InChI=1S/C29H40O4/c1-2-3-4-5-6-7-8-9-10-16-24-32-28(30)22-17-23-29(31)33-27-21-15
InchiKey: NYNJQAAAHMMATE-UHFFFAOYSA-N
Formula: C29H40O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1-c1ccccc1
Mol. weight [g/mol]: 452.63

Physical Properties

Property code	Value	Unit	Source
gf	-59.35	kJ/mol	Joback Method
hf	-669.90	kJ/mol	Joback Method
hfus	64.13	kJ/mol	Joback Method
hvap	103.67	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	7.893		Crippen Method
mcvol	386.830	ml/mol	McGowan Method
pc	939.22	kPa	Joback Method
rinpol	3422.00		NIST Webbook
tb	1073.84	K	Joback Method
tc	1315.50	K	Joback Method
tf	626.27	K	Joback Method
vc	1.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1322.46	J/mol×K	1073.84	Joback Method
cpg	1337.42	J/mol×K	1114.12	Joback Method
cpg	1350.72	J/mol×K	1154.39	Joback Method
cpg	1362.43	J/mol×K	1194.67	Joback Method
cpg	1372.67	J/mol×K	1234.94	Joback Method
cpg	1381.51	J/mol×K	1275.22	Joback Method
cpg	1389.06	J/mol×K	1315.50	Joback Method
dvisc	0.0001861	Pa×s	626.27	Joback Method
dvisc	0.0000977	Pa×s	700.87	Joback Method

dvisc	0.0000580	Pa×s	775.46	Joback Method
dvisc	0.0000378	Pa×s	850.05	Joback Method
dvisc	0.0000264	Pa×s	924.65	Joback Method
dvisc	0.0000194	Pa×s	999.24	Joback Method
dvisc	0.0000149	Pa×s	1073.84	Joback Method

Sources

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=U358976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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