

Glutaric acid, hept-2-yl 4-biphenyl ester

Inchi: InChI=1S/C24H30O4/c1-3-4-6-10-19(2)27-23(25)13-9-14-24(26)28-22-17-15-21(16-18-2
InchiKey: MXRSAKRMUBSTES-UHFFFAOYSA-N
Formula: C24H30O4
SMILES: CCCCCC(C)OC(=O)CCCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 382.49

Physical Properties

Property code	Value	Unit	Source
gf	-103.89	kJ/mol	Joback Method
hf	-571.98	kJ/mol	Joback Method
hfus	47.66	kJ/mol	Joback Method
hvap	92.16	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	5.941		Crippen Method
mvol	316.380	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2947.00		NIST Webbook
rinpol	2947.00		NIST Webbook
tb	959.00	K	Joback Method
tc	1183.19	K	Joback Method
tf	554.92	K	Joback Method
vc	1.206	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.17	J/molxK	959.00	Joback Method
cpg	1031.66	J/molxK	996.37	Joback Method
cpg	1044.74	J/molxK	1033.73	Joback Method
cpg	1056.47	J/molxK	1071.10	Joback Method
cpg	1066.89	J/molxK	1108.46	Joback Method
cpg	1076.05	J/molxK	1145.83	Joback Method
cpg	1084.02	J/molxK	1183.19	Joback Method
dvisc	0.0003715	Paxs	554.92	Joback Method

dvisc	0.0001929	Paxs	622.27	Joback Method
dvisc	0.0001139	Paxs	689.61	Joback Method
dvisc	0.0000738	Paxs	756.96	Joback Method
dvisc	0.0000514	Paxs	824.31	Joback Method
dvisc	0.0000377	Paxs	891.65	Joback Method
dvisc	0.0000290	Paxs	959.00	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=U390125&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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