

Glutaric acid, 2-biphenyl isoheptyl ester

Inchi:	InChI=1S/C23H28O4/c1-18(2)10-9-17-26-22(24)15-8-16-23(25)27-21-14-7-6-13-20(21)1
InchiKey:	WGTFKSJYHUJWGI-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	CC(C)CCCOC(=O)CCCC(=O)Oc1ccccc1-c1ccccc1
Mol. weight [g/mol]:	368.47

Physical Properties

Property code	Value	Unit	Source
gf	-112.31	kJ/mol	Joback Method
hf	-551.34	kJ/mol	Joback Method
hfus	45.07	kJ/mol	Joback Method
hvap	89.93	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	5.409		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpola	2736.00		NIST Webbook
tb	936.12	K	Joback Method
tc	1159.77	K	Joback Method
tf	543.65	K	Joback Method
vc	1.149	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.46	J/molxK	936.12	Joback Method
cpg	1016.46	J/molxK	1122.49	Joback Method
cpg	1007.23	J/molxK	1085.22	Joback Method
cpg	996.76	J/molxK	1047.94	Joback Method
cpg	985.01	J/molxK	1010.67	Joback Method
cpg	971.93	J/molxK	973.39	Joback Method
cpg	1024.50	J/molxK	1159.77	Joback Method
dvisc	0.0000335	Paxs	936.12	Joback Method
dvisc	0.0000436	Paxs	870.71	Joback Method

dvisc	0.0000591	Paxs	805.30	Joback Method
dvisc	0.0000846	Paxs	739.88	Joback Method
dvisc	0.0001298	Paxs	674.47	Joback Method
dvisc	0.0002184	Paxs	609.06	Joback Method
dvisc	0.0004164	Paxs	543.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358969&Units=SI
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

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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