

Glutaric acid, di(3-phenylpropyl) ester

Inchi:	InChI=1S/C23H28O4/c24-22(26-18-8-14-20-10-3-1-4-11-20)16-7-17-23(25)27-19-9-15-2
InchiKey:	HLWIUNZETPJEV-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	O=C(CCCC(=O)OCCc1ccccc1)OCCc1ccccc1
Mol. weight [g/mol]:	368.47

Physical Properties

Property code	Value	Unit	Source
gf	-100.24	kJ/mol	Joback Method
hf	-534.59	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	89.66	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.509		Crippen Method
mvol	302.290	ml/mol	McGowan Method
pc	1400.64	kPa	Joback Method
rinpol	3052.00		NIST Webbook
rinpol	3052.00		NIST Webbook
tb	931.58	K	Joback Method
tc	1152.51	K	Joback Method
tf	546.13	K	Joback Method
vc	1.155	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.01	J/molxK	931.58	Joback Method
cpg	972.52	J/molxK	968.40	Joback Method
cpg	985.70	J/molxK	1005.22	Joback Method
cpg	997.60	J/molxK	1042.04	Joback Method
cpg	1008.29	J/molxK	1078.87	Joback Method
cpg	1017.81	J/molxK	1115.69	Joback Method
cpg	1026.22	J/molxK	1152.51	Joback Method
dvisc	0.0004322	Paxs	546.13	Joback Method

dvisc	0.0002297	Paxs	610.37	Joback Method
dvisc	0.0001377	Paxs	674.61	Joback Method
dvisc	0.0000902	Paxs	738.86	Joback Method
dvisc	0.0000633	Paxs	803.10	Joback Method
dvisc	0.0000468	Paxs	867.34	Joback Method
dvisc	0.0000360	Paxs	931.58	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=U360144&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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