

Glutaric acid, di(1-phenylpropyl) ester

Inchi:	InChI=1S/C23H28O4/c1-3-20(18-12-7-5-8-13-18)26-22(24)16-11-17-23(25)27-21(4-2)19
InchiKey:	FMSQSJWGXTVTPC-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	CCC(OC(=O)CCCC(=O)OC(CC)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	368.47

Physical Properties

Property code	Value	Unit	Source
gf	-105.12	kJ/mol	Joback Method
hf	-545.15	kJ/mol	Joback Method
hfus	41.94	kJ/mol	Joback Method
hvap	88.88	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.546		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinqol	2688.00		NIST Webbook
tb	930.70	K	Joback Method
tc	1155.57	K	Joback Method
tf	516.13	K	Joback Method
vc	1.143	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.95	J/molxK	930.70	Joback Method
cpg	973.63	J/molxK	968.18	Joback Method
cpg	986.90	J/molxK	1005.66	Joback Method
cpg	998.83	J/molxK	1043.14	Joback Method
cpg	1009.46	J/molxK	1080.62	Joback Method
cpg	1018.87	J/molxK	1118.10	Joback Method
cpg	1027.10	J/molxK	1155.57	Joback Method
dvisc	0.0005427	Paxs	516.13	Joback Method
dvisc	0.0002519	Paxs	585.23	Joback Method

dvisc	0.0001375	Paxs	654.32	Joback Method
dvisc	0.0000843	Paxs	723.42	Joback Method
dvisc	0.0000562	Paxs	792.51	Joback Method
dvisc	0.0000400	Paxs	861.61	Joback Method
dvisc	0.0000300	Paxs	930.70	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=U358963&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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