

Glutaric acid, butyl 1-phenyl-2-(3-cyclohexenyl)ethyl ester

Inchi:	InChI=1S/C23H32O4/c1-2-3-17-26-22(24)15-10-16-23(25)27-21(20-13-8-5-9-14-20)18-1
InchiKey:	MFRUAQQLDFSFKW-UHFFFAOYSA-N
Formula:	C23H32O4
SMILES:	CCCCOC(=O)CCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]:	372.50

Physical Properties

Property code	Value	Unit	Source
gf	-160.68	kJ/mol	Joback Method
hf	-664.30	kJ/mol	Joback Method
hfus	44.47	kJ/mol	Joback Method
hvap	87.71	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.531		Crippen Method
mcvol	310.890	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinqol	2741.00		NIST Webbook
tb	923.17	K	Joback Method
tc	1143.17	K	Joback Method
tf	512.85	K	Joback Method
vc	1.177	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.30	J/molxK	923.17	Joback Method
cpg	1040.63	J/molxK	959.84	Joback Method
cpg	1055.42	J/molxK	996.50	Joback Method
cpg	1068.72	J/molxK	1033.17	Joback Method
cpg	1080.59	J/molxK	1069.84	Joback Method
cpg	1091.09	J/molxK	1106.50	Joback Method
cpg	1100.25	J/molxK	1143.17	Joback Method
dvisc	0.0006331	Paxs	512.85	Joback Method
dvisc	0.0002961	Paxs	581.24	Joback Method

dvisc	0.0001625	Paxs	649.62	Joback Method
dvisc	0.0001000	Paxs	718.01	Joback Method
dvisc	0.0000669	Paxs	786.40	Joback Method
dvisc	0.0000478	Paxs	854.78	Joback Method
dvisc	0.0000359	Paxs	923.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358586&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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