

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

Inchi:	InChI=1S/C22H30O4/c1-2-16-25-21(23)14-9-15-22(24)26-20(19-12-7-4-8-13-19)17-18-1
InchiKey:	YDGKRZASURGGEY-UHFFFAOYSA-N
Formula:	C22H30O4
SMILES:	CCCOC(=O)CCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]:	358.47

Physical Properties

Property code	Value	Unit	Source
gf	-169.10	kJ/mol	Joback Method
hf	-643.66	kJ/mol	Joback Method
hfus	41.88	kJ/mol	Joback Method
hvap	85.49	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.141		Crippen Method
mvol	296.800	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2643.00		NIST Webbook
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tb	900.29	K	Joback Method
tc	1120.38	K	Joback Method
tf	501.58	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.11	J/molxK	900.29	Joback Method
cpg	1031.42	J/molxK	1083.70	Joback Method
cpg	1020.79	J/molxK	1047.02	Joback Method
cpg	1008.79	J/molxK	1010.33	Joback Method
cpg	995.38	J/molxK	973.65	Joback Method
cpg	980.50	J/molxK	936.97	Joback Method
cpg	1040.73	J/molxK	1120.38	Joback Method
dvisc	0.0000416	Paxs	900.29	Joback Method

dvisc	0.0000553	Paxs	833.84	Joback Method
dvisc	0.0000772	Paxs	767.39	Joback Method
dvisc	0.0001149	Paxs	700.93	Joback Method
dvisc	0.0001858	Paxs	634.48	Joback Method
dvisc	0.0003363	Paxs	568.03	Joback Method
dvisc	0.0007124	Paxs	501.58	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=U358584&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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