

Glutaric acid, cyclohexylmethyl 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C21H30O5/c1-16(2)25-18-11-6-7-12-19(18)26-21(23)14-8-13-20(22)24-15-17-
InchiKey:	UZFIAJJCXGZJBK-UHFFFAOYSA-N
Formula:	C21H30O5
SMILES:	CC(C)Oc1ccccc1OC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	362.46

Physical Properties

Property code	Value	Unit	Source
gf	-322.11	kJ/mol	Joback Method
hf	-824.49	kJ/mol	Joback Method
hfus	38.87	kJ/mol	Joback Method
hvap	86.04	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.673		Crippen Method
mcvol	292.880	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	2645.00		NIST Webbook
tb	905.65	K	Joback Method
tc	1126.16	K	Joback Method
tf	524.30	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.15	J/molxK	905.65	Joback Method
cpg	978.31	J/molxK	942.40	Joback Method
cpg	992.82	J/molxK	979.15	Joback Method
cpg	1005.70	J/molxK	1015.90	Joback Method
cpg	1016.97	J/molxK	1052.65	Joback Method
cpg	1026.65	J/molxK	1089.41	Joback Method
cpg	1034.76	J/molxK	1126.16	Joback Method
dvisc	0.0004710	Paxs	524.30	Joback Method
dvisc	0.0002389	Paxs	587.86	Joback Method

dvisc	0.0001384	Paxs	651.42	Joback Method
dvisc	0.0000883	Paxs	714.97	Joback Method
dvisc	0.0000607	Paxs	778.53	Joback Method
dvisc	0.0000441	Paxs	842.09	Joback Method
dvisc	0.0000335	Paxs	905.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391874&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

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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