

Glutaric acid, isohexyl 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C20H30O5/c1-15(2)9-8-14-23-19(21)12-7-13-20(22)25-18-11-6-5-10-17(18)24
InchiKey:	XNWFJSSCSREYOY-UHFFFAOYSA-N
Formula:	C20H30O5
SMILES:	CC(C)CCCOC(=O)CCCC(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]:	350.45

Physical Properties

Property code	Value	Unit	Source
gf	-357.42	kJ/mol	Joback Method
hf	-863.45	kJ/mol	Joback Method
hfus	40.92	kJ/mol	Joback Method
hvap	83.00	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.529		Crippen Method
mvol	289.650	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	862.78	K	Joback Method
tc	1067.37	K	Joback Method
tf	490.65	K	Joback Method
vc	1.101	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.12	J/molxK	862.78	Joback Method
cpg	974.74	J/molxK	1033.27	Joback Method
cpg	963.92	J/molxK	999.17	Joback Method
cpg	951.85	J/molxK	965.07	Joback Method
cpg	938.54	J/molxK	930.98	Joback Method
cpg	923.97	J/molxK	896.88	Joback Method
cpg	984.34	J/molxK	1067.37	Joback Method
dvisc	0.0000344	Paxs	862.78	Joback Method

dvisc	0.0000455	Paxs	800.76	Joback Method
dvisc	0.0000631	Paxs	738.74	Joback Method
dvisc	0.0000928	Paxs	676.72	Joback Method
dvisc	0.0001476	Paxs	614.69	Joback Method
dvisc	0.0002604	Paxs	552.67	Joback Method
dvisc	0.0005303	Paxs	490.65	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=U358573&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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