

Glutaric acid, 2-methylpent-3-yl 1-phenylpropyl ester

Inchi:	InChI=1S/C20H30O4/c1-5-17(15(3)4)23-19(21)13-10-14-20(22)24-18(6-2)16-11-8-7-9-12
InchiKey:	BESLUQNCWHHHTF-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCC(OC(=O)CCCC(=O)OC(CC)C(C)C)c1ccccc1
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-245.23	kJ/mol	Joback Method
hf	-725.04	kJ/mol	Joback Method
hfus	36.60	kJ/mol	Joback Method
hvap	79.54	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.829		Crippen Method
mvol	283.780	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	834.94	K	Joback Method
tc	1039.78	K	Joback Method
tf	440.90	K	Joback Method
vc	1.077	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.88	J/molxK	834.94	Joback Method
cpg	896.53	J/molxK	869.08	Joback Method
cpg	911.95	J/molxK	903.22	Joback Method
cpg	926.18	J/molxK	937.36	Joback Method
cpg	939.24	J/molxK	971.50	Joback Method
cpg	951.17	J/molxK	1005.64	Joback Method
cpg	961.99	J/molxK	1039.78	Joback Method
dvisc	0.0011245	Paxs	440.90	Joback Method

dvisc	0.0004550	Paxs	506.57	Joback Method
dvisc	0.0002266	Paxs	572.25	Joback Method
dvisc	0.0001303	Paxs	637.92	Joback Method
dvisc	0.0000830	Paxs	703.59	Joback Method
dvisc	0.0000572	Paxs	769.27	Joback Method
dvisc	0.0000417	Paxs	834.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392046&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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