

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

Inchi:	InChI=1S/C19H28O4/c1-5-17(16-10-7-6-8-11-16)23-19(21)13-9-12-18(20)22-15(4)14(2)3
InchiKey:	RGZNQFLPFBKMG-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CCC(OC(=O)CCCC(=O)OC(C)C(C)C)c1ccccc1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-253.65	kJ/mol	Joback Method
hf	-704.40	kJ/mol	Joback Method
hfus	34.01	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.439		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinqol	2135.00		NIST Webbook
tb	812.06	K	Joback Method
tc	1017.36	K	Joback Method
tf	429.63	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.29	J/molxK	812.06	Joback Method
cpg	837.81	J/molxK	846.28	Joback Method
cpg	853.13	J/molxK	880.49	Joback Method
cpg	867.29	J/molxK	914.71	Joback Method
cpg	880.31	J/molxK	948.93	Joback Method
cpg	892.22	J/molxK	983.15	Joback Method
cpg	903.04	J/molxK	1017.36	Joback Method
dvisc	0.0012680	Paxs	429.63	Joback Method
dvisc	0.0005171	Paxs	493.37	Joback Method

dvisc	0.0002589	Paxs	557.11	Joback Method
dvisc	0.0001494	Paxs	620.85	Joback Method
dvisc	0.0000955	Paxs	684.58	Joback Method
dvisc	0.0000659	Paxs	748.32	Joback Method
dvisc	0.0000482	Paxs	812.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392045&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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