Glutaric acid, 2-methylpent-3-yl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C19H28O4/c1-6-16(13(2)3)22-18(20)11-8-12-19(21)23-17-10-7-9-14(4)15(17)5

InchiKey: SLBWVGLDABUOKB-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CCC(OC(=O)CCCC(=O)Oc1cccc(C)c1C)C(C)C

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-270.47	kJ/mol	Joback Method
hf	-722.06	kJ/mol	Joback Method
hfus	36.76	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.357		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2255.00		NIST Webbook
tb	822.46	K	Joback Method
tc	1027.04	K	Joback Method
tf	469.67	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.45	J/mol×K	822.46	Joback Method
cpg	835.59	J/mol×K	856.56	Joback Method
cpg	850.58	J/mol×K	890.65	Joback Method
cpg	864.43	J/mol×K	924.75	Joback Method
cpg	877.17	J/mol×K	958.85	Joback Method
cpg	888.80	J/mol×K	992.95	Joback Method
cpg	899.33	J/mol×K	1027.04	Joback Method
dvisc	0.0007180	Pa×s	469.67	Joback Method
dvisc	0.0003662	Pa×s	528.47	Joback Method

dvisc	0.0002137	Pa×s	587.27	Joback Method
dvisc	0.0001376	Pa×s	646.07	Joback Method
dvisc	0.0000953	Pa×s	704.86	Joback Method
dvisc	0.0000699	Pa×s	763.66	Joback Method
dvisc	0.0000535	Pa×s	822.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U392216&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