Glutaric acid, cyclohexylmethyl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C20H28O4/c1-15-8-6-11-18(16(15)2)24-20(22)13-7-12-19(21)23-14-17-9-4-3-5

InchiKey: KLRYPRLQCNNICL-UHFFFAOYSA-N

Formula: C20H28O4

SMILES: Cc1cccc(OC(=O)CCCC(=O)OCC2CCCCC2)c1C

Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-232.72	kJ/mol	Joback Method
hf	-677.82	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	82.45	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.503		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1550.00	kPa	Joback Method
rinpol	2603.00		NIST Webbook
rinpol	2603.00		NIST Webbook
tb	865.77	K	Joback Method
tc	1085.78	K	Joback Method
tf	518.32	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.20	J/mol×K	865.77	Joback Method
cpg	889.04	J/mol×K	902.44	Joback Method
cpg	904.39	J/mol×K	939.11	Joback Method
cpg	918.27	J/mol×K	975.77	Joback Method
cpg	930.72	J/mol×K	1012.44	Joback Method
cpg	941.74	J/mol×K	1049.11	Joback Method
cpg	951.38	J/mol×K	1085.78	Joback Method
dvisc	0.0005810	Pa×s	518.32	Joback Method

dvisc	0.0003257	Pa×s	576.23	Joback Method
dvisc	0.0002029	Pa×s	634.14	Joback Method
dvisc	0.0001368	Pa×s	692.04	Joback Method
dvisc	0.0000981	Pa×s	749.95	Joback Method
dvisc	0.0000737	Pa×s	807.86	Joback Method
dvisc	0.0000576	Pa×s	865.77	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=U392223&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