Glutaric acid, 2-ethylhexyl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C21H32O4/c1-5-7-11-18(6-2)15-24-20(22)13-9-14-21(23)25-19-12-8-10-16(3)1

InchiKey: KXOIFRUPFKMKHJ-UHFFFAOYSA-N

Formula: C21H32O4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-251.19	kJ/mol	Joback Method
hf	-758.06	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	83.86	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.139		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	868.66	K	Joback Method
tc	1072.18	K	Joback Method
tf	507.21	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.05	J/mol×K	868.66	Joback Method
cpg	953.40	J/mol×K	902.58	Joback Method
cpg	968.55	J/mol×K	936.50	Joback Method
cpg	982.50	J/mol×K	970.42	Joback Method
cpg	995.28	J/mol×K	1004.34	Joback Method
cpg	1006.91	J/mol×K	1038.26	Joback Method
cpg	1017.41	J/mol×K	1072.18	Joback Method
dvisc	0.0005155	Pa×s	507.21	Joback Method

dvisc	0.0002755	Pa×s	567.45	Joback Method
dvisc	0.0001661	Pa×s	627.69	Joback Method
dvisc	0.0001094	Pa×s	687.93	Joback Method
dvisc	0.0000771	Pa×s	748.18	Joback Method
dvisc	0.0000572	Pa×s	808.42	Joback Method
dvisc	0.0000442	Pa×s	868.66	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=U392222&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