Glutaric acid, 3,5-dimethylphenyl ethyl ester

Inchi: InChI=1S/C15H20O4/c1-4-18-14(16)6-5-7-15(17)19-13-9-11(2)8-12(3)10-13/h8-10H,4-7
InchiKey: FPOUGJRHQLASBT-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: CCOC(=O)CCCC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	-299.27	kJ/mol	Joback Method
hf	-628.94	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	70.90	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.942		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	2005.00		NIST Webbook
rinpol	2005.00		NIST Webbook
tb	731.82	K	Joback Method
tc	936.25	K	Joback Method
tf	454.59	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.78	J/mol×K	731.82	Joback Method
cpg	656.98	J/mol×K	902.18	Joback Method
cpg	645.96	J/mol×K	868.11	Joback Method
cpg	634.03	J/mol×K	834.04	Joback Method
cpg	621.19	J/mol×K	799.96	Joback Method
cpg	607.44	J/mol×K	765.89	Joback Method
cpg	667.10	J/mol×K	936.25	Joback Method
dvisc	0.0001058	Pa×s	731.82	Joback Method

dvisc	0.0001319	Pa×s	685.62	Joback Method
dvisc	0.0001697	Pa×s	639.41	Joback Method
dvisc	0.0002270	Pa×s	593.21	Joback Method
dvisc	0.0003191	Pa×s	547.00	Joback Method
dvisc	0.0004776	Pa×s	500.80	Joback Method
dvisc	0.0007757	Pa×s	454.59	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=U358695&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

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