Glutaric acid, 3-methylbut-2-en-1-yl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C18H24O4/c1-13(2)11-12-21-17(19)9-6-10-18(20)22-16-8-5-7-14(3)15(16)4/h5

InchiKey: YZFQVHVDBCHZKC-UHFFFAOYSA-N

Formula: C18H24O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-202.34	kJ/mol	Joback Method
hf	-583.43	kJ/mol	Joback Method
hfus	40.10	kJ/mol	Joback Method
hvap	77.61	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.889		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	2284.00		NIST Webbook
rinpol	2284.00		NIST Webbook
tb	804.50	K	Joback Method
tc	1012.38	K	Joback Method
tf	469.36	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.52	J/mol×K	804.50	Joback Method
cpg	749.77	J/mol×K	839.15	Joback Method
cpg	763.99	J/mol×K	873.79	Joback Method
cpg	777.22	J/mol×K	908.44	Joback Method
cpg	789.47	J/mol×K	943.08	Joback Method
cpg	800.77	J/mol×K	977.73	Joback Method
cpg	811.15	J/mol×K	1012.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392217&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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