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

Inchi: InChI=1S/C18H26O4/c1-12(2)15(5)21-17(19)10-7-11-18(20)22-16-9-6-8-13(3)14(16)4/h6
InchiKey: ABWRSBLINMBELB-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: Cc1cccc(OC(=O)CCCC(=O)OC(C)C(C)C)c1C
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-278.89	kJ/mol	Joback Method
hf	-701.42	kJ/mol	Joback Method
hfus	34.17	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.967		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	2173.00		NIST Webbook
rinpol	2173.00		NIST Webbook
tb	799.58	K	Joback Method
tc	1004.92	K	Joback Method
tf	458.40	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.61	J/mol×K	799.58	Joback Method
cpg	830.40	J/mol×K	970.70	Joback Method
cpg	818.82	J/mol×K	936.47	Joback Method
cpg	806.16	J/mol×K	902.25	Joback Method
cpg	792.41	J/mol×K	868.03	Joback Method
cpg	777.56	J/mol×K	833.80	Joback Method
cpg	840.92	J/mol×K	1004.92	Joback Method
dvisc	0.0000613	Pa×s	799.58	Joback Method

dvisc	0.0000798	Pa×s	742.72	Joback Method
dvisc	0.0001084	Pa×s	685.85	Joback Method
dvisc	0.0001557	Pa×s	628.99	Joback Method
dvisc	0.0002404	Pa×s	572.13	Joback Method
dvisc	0.0004085	Pa×s	515.26	Joback Method
dvisc	0.0007916	Pa×s	458.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392215&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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