

Glutaric acid, di(2,3-dimethylphenyl) ester

Inchi: InChI=1S/C21H24O4/c1-14-8-5-10-18(16(14)3)24-20(22)12-7-13-21(23)25-19-11-6-9-15
InchiKey: GDXGEHBHDPJIDH-UHFFFAOYSA-N
Formula: C21H24O4
SMILES: Cc1cccc(OC(=O)CCCC(=O)Oc2cccc(C)c2C)c1C
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-155.60	kJ/mol	Joback Method
hf	-539.19	kJ/mol	Joback Method
hfus	42.25	kJ/mol	Joback Method
hvap	87.85	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.602		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1550.00	kPa	Joback Method
rinpol	2819.00		NIST Webbook
rinpol	2819.00		NIST Webbook
tb	905.74	K	Joback Method
tc	1130.44	K	Joback Method
tf	573.67	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.99	J/mol×K	905.74	Joback Method
cpg	849.94	J/mol×K	943.19	Joback Method
cpg	862.56	J/mol×K	980.64	Joback Method
cpg	873.86	J/mol×K	1018.09	Joback Method
cpg	883.86	J/mol×K	1055.54	Joback Method
cpg	892.58	J/mol×K	1092.99	Joback Method
cpg	900.04	J/mol×K	1130.44	Joback Method
dvisc	0.0003269	Pa×s	573.67	Joback Method

dvisc	0.0002100	Pa×s	629.02	Joback Method
dvisc	0.0001449	Pa×s	684.36	Joback Method
dvisc	0.0001057	Pa×s	739.71	Joback Method
dvisc	0.0000805	Pa×s	795.05	Joback Method
dvisc	0.0000636	Pa×s	850.39	Joback Method
dvisc	0.0000517	Pa×s	905.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359313&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
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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