Glutaric acid, 3-methylbut-2-yl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C18H26O5/c1-12(2)14(4)22-17(19)7-6-8-18(20)23-16-11-13(3)9-10-15(16)21-5

InchiKey: CZEMBKSEAODHFV-UHFFFAOYSA-N

Formula: C18H26O5

SMILES: COc1ccc(C)cc1OC(=O)CCCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-383.89	kJ/mol	Joback Method
hf	-833.64	kJ/mol	Joback Method
hfus	35.35	kJ/mol	Joback Method
hvap	79.21	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.667		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	822.00	K	Joback Method
tc	1027.16	K	Joback Method
tf	480.63	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.30	J/mol×K	822.00	Joback Method
cpg	805.77	J/mol×K	856.19	Joback Method
cpg	820.06	J/mol×K	890.39	Joback Method
cpg	833.18	J/mol×K	924.58	Joback Method
cpg	845.13	J/mol×K	958.77	Joback Method
cpg	855.90	J/mol×K	992.96	Joback Method
cpg	865.50	J/mol×K	1027.16	Joback Method
dvisc	0.0005532	Pa×s	480.63	Joback Method

dvisc	0.0002940	Pa×s	537.52	Joback Method
dvisc	0.0001763	Pa×s	594.42	Joback Method
dvisc	0.0001156	Pa×s	651.32	Joback Method
dvisc	0.0000812	Pa×s	708.21	Joback Method
dvisc	0.0000600	Pa×s	765.11	Joback Method
dvisc	0.0000463	Pa×s	822.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393921&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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