Glutaric acid, 3-methylbenzyl propyl ester

Inchi: InChI=1S/C16H22O4/c1-3-10-19-15(17)8-5-9-16(18)20-12-14-7-4-6-13(2)11-14/h4,6-7,1
InchiKey: MZGKDTFTSHWNEX-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CCCOC(=O)CCCC(=O)OCc1cccc(C)c1
Mol. weight [g/mol]: 278.34

Physical Properties

Property code	Value	Unit	Source
gf	-281.22	kJ/mol	Joback Method
hf	-638.11	kJ/mol	Joback Method
hfus	36.42	kJ/mol	Joback Method
hvap	72.46	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.162		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	2287.00		NIST Webbook
tb	749.72	K	Joback Method
tc	951.49	K	Joback Method
tf	453.34	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.45	J/mol×K	749.72	Joback Method
cpg	663.58	J/mol×K	783.35	Joback Method
cpg	677.73	J/mol×K	816.98	Joback Method
cpg	690.92	J/mol×K	850.61	Joback Method
cpg	703.17	J/mol×K	884.24	Joback Method
cpg	714.48	J/mol×K	917.86	Joback Method
cpg	724.87	J/mol×K	951.49	Joback Method
dvisc	0.0008522	Pa×s	453.34	Joback Method
dvisc	0.0004919	Pa×s	502.74	Joback Method

dvisc	0.0003132	Pa×s	552.13	Joback Method
dvisc	0.0002148	Pa×s	601.53	Joback Method
dvisc	0.0001560	Pa×s	650.93	Joback Method
dvisc	0.0001185	Pa×s	700.32	Joback Method
dvisc	0.0000934	Pa×s	749.72	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=U377646&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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