Glutaric acid, octyl 1-phenylpropyl ester

Inchi: InChI=1S/C22H34O4/c1-3-5-6-7-8-12-18-25-21(23)16-13-17-22(24)26-20(4-2)19-14-10-9
InchiKey: FQRWTNPCBLINQZ-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CCCCCCCCOC(=O)CCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-223.51	kJ/mol	Joback Method
hf	-755.76	kJ/mol	Joback Method
hfus	48.83	kJ/mol	Joback Method
hvap	84.77	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.755		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	881.58	K	Joback Method
tc	1084.93	K	Joback Method
tf	493.44	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.33	J/mol×K	881.58	Joback Method
cpg	1015.04	J/mol×K	915.47	Joback Method
cpg	1030.51	J/mol×K	949.36	Joback Method
cpg	1044.77	J/mol×K	983.26	Joback Method
cpg	1057.86	J/mol×K	1017.15	Joback Method
cpg	1069.80	J/mol×K	1051.04	Joback Method
cpg	1080.63	J/mol×K	1084.93	Joback Method
dvisc	0.0006396	Pa×s	493.44	Joback Method

dvisc	0.0003024	Pa×s	558.13	Joback Method
dvisc	0.0001670	Pa×s	622.82	Joback Method
dvisc	0.0001031	Pa×s	687.51	Joback Method
dvisc	0.0000692	Pa×s	752.20	Joback Method
dvisc	0.0000495	Pa×s	816.89	Joback Method
dvisc	0.0000371	Pa×s	881.58	Joback Method

Sources

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=U358955&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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