

Glutaric acid, octyl 3-phenylprop-2-enyl ester

Inchi: InChI=1S/C22H32O4/c1-2-3-4-5-6-10-18-25-21(23)16-11-17-22(24)26-19-12-15-20-13-8
InchiKey: CLLYWQGFKCZJQO-NTCAYCPXSA-N
Formula: C22H32O4
SMILES: CCCCCCOC(=O)CCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-140.85	kJ/mol	Joback Method
hf	-633.26	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	85.11	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.317		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpola	2813.00		NIST Webbook
tb	886.18	K	Joback Method
tc	1091.44	K	Joback Method
tf	503.36	K	Joback Method
vc	1.188	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.69	J/molxK	886.18	Joback Method
cpg	1040.76	J/molxK	1057.23	Joback Method
cpg	1028.84	J/molxK	1023.02	Joback Method
cpg	1015.92	J/molxK	988.81	Joback Method
cpg	1001.96	J/molxK	954.60	Joback Method
cpg	986.89	J/molxK	920.39	Joback Method
cpg	1051.72	J/molxK	1091.44	Joback Method
dvisc	0.0000355	Paxs	886.18	Joback Method
dvisc	0.0000467	Paxs	822.38	Joback Method

dvisc	0.0000642	Paxs	758.57	Joback Method
dvisc	0.0000938	Paxs	694.77	Joback Method
dvisc	0.0001479	Paxs	630.97	Joback Method
dvisc	0.0002584	Paxs	567.16	Joback Method
dvisc	0.0005199	Paxs	503.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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