

Glutaric acid, heptyl 1-phenylpropyl ester

Inchi:	InChI=1S/C21H32O4/c1-3-5-6-7-11-17-24-20(22)15-12-16-21(23)25-19(4-2)18-13-9-8-10
InchiKey:	STIRUQHTDAQHTB-UHFFFAOYSA-N
Formula:	C21H32O4
SMILES:	CCCCCCCOC(=O)CCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]:	348.48

Physical Properties

Property code	Value	Unit	Source
gf	-231.93	kJ/mol	Joback Method
hf	-735.12	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	82.54	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.365		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinqol	2481.00		NIST Webbook
tb	858.70	K	Joback Method
tc	1060.45	K	Joback Method
tf	482.17	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.24	J/molxK	858.70	Joback Method
cpg	954.76	J/molxK	892.33	Joback Method
cpg	970.10	J/molxK	925.95	Joback Method
cpg	984.26	J/molxK	959.58	Joback Method
cpg	997.29	J/molxK	993.20	Joback Method
cpg	1009.22	J/molxK	1026.83	Joback Method
cpg	1020.07	J/molxK	1060.45	Joback Method
dvisc	0.0007178	Paxs	482.17	Joback Method
dvisc	0.0003427	Paxs	544.92	Joback Method

dvisc	0.0001906	Paxs	607.68	Joback Method
dvisc	0.0001183	Paxs	670.43	Joback Method
dvisc	0.0000797	Paxs	733.19	Joback Method
dvisc	0.0000571	Paxs	795.94	Joback Method
dvisc	0.0000430	Paxs	858.70	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=U358954&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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