

Glutaric acid, heptyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C21H32O5/c1-4-5-6-7-10-16-24-20(22)14-11-15-21(23)26-19-13-9-8-12-18(19)
InchiKey: XEWPXNMZODLXBB-UHFFFAOYSA-N
Formula: C21H32O5
SMILES: CCCCCCOC(=O)CCCC(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-346.56	kJ/mol	Joback Method
hf	-878.81	kJ/mol	Joback Method
hfus	47.04	kJ/mol	Joback Method
hvap	85.61	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.063		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	2575.00		NIST Webbook
tb	886.10	K	Joback Method
tc	1090.63	K	Joback Method
tf	516.92	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.23	J/molxK	886.10	Joback Method
cpg	983.12	J/molxK	920.19	Joback Method
cpg	997.70	J/molxK	954.28	Joback Method
cpg	1011.00	J/molxK	988.37	Joback Method
cpg	1023.03	J/molxK	1022.46	Joback Method
cpg	1033.79	J/molxK	1056.54	Joback Method
cpg	1043.30	J/molxK	1090.63	Joback Method
dvisc	0.0004176	Paxs	516.92	Joback Method
dvisc	0.0002177	Paxs	578.45	Joback Method

dvisc	0.0001286	Paxs	639.98	Joback Method
dvisc	0.0000833	Paxs	701.51	Joback Method
dvisc	0.0000579	Paxs	763.04	Joback Method
dvisc	0.0000425	Paxs	824.57	Joback Method
dvisc	0.0000325	Paxs	886.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358575&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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