

Glutaric acid, dec-2-yl 4-acetylphenyl ester

Inchi: InChI=1S/C23H34O5/c1-4-5-6-7-8-9-11-18(2)27-22(25)12-10-13-23(26)28-21-16-14-20(1)
InchiKey: XWBUAKSNOZBJDB-UHFFFAOYSA-N
Formula: C23H34O5
SMILES: CCCCCCCC(C)OC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 390.51

Physical Properties

Property code	Value	Unit	Source
gf	-353.64	kJ/mol	Joback Method
hf	-900.45	kJ/mol	Joback Method
hfus	52.63	kJ/mol	Joback Method
hvap	94.40	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.647		Crippen Method
mvol	327.620	ml/mol	McGowan Method
pc	1151.44	kPa	Joback Method
rinpol	2901.00		NIST Webbook
rinpol	2901.00		NIST Webbook
tb	963.31	K	Joback Method
tc	1180.32	K	Joback Method
tf	567.16	K	Joback Method
vc	1.264	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1073.90	J/molxK	963.31	Joback Method
cpg	1088.75	J/molxK	999.48	Joback Method
cpg	1102.18	J/molxK	1035.65	Joback Method
cpg	1114.25	J/molxK	1071.82	Joback Method
cpg	1124.97	J/molxK	1107.99	Joback Method
cpg	1134.39	J/molxK	1144.15	Joback Method
cpg	1142.54	J/molxK	1180.32	Joback Method
dvisc	0.0003833	Paxs	567.16	Joback Method

dvisc	0.0002022	Paxs	633.19	Joback Method
dvisc	0.0001203	Paxs	699.21	Joback Method
dvisc	0.0000783	Paxs	765.24	Joback Method
dvisc	0.0000546	Paxs	831.26	Joback Method
dvisc	0.0000401	Paxs	897.28	Joback Method
dvisc	0.0000308	Paxs	963.31	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392037&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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