

Glutaric acid, 1-cyclopentylethyl dec-2-yl ester

Inchi: InChI=1S/C22H40O4/c1-4-5-6-7-8-9-13-18(2)25-21(23)16-12-17-22(24)26-19(3)20-14-10
InchiKey: JLJSNSJHFUHRMS-UHFFFAOYSA-N
Formula: C22H40O4
SMILES: CCCCCCCC(C)OC(=O)CCCC(=O)OC(C)C1CCCC1
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-301.81	kJ/mol	Joback Method
hf	-937.09	kJ/mol	Joback Method
hfus	45.20	kJ/mol	Joback Method
hvap	82.36	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.961		Crippen Method
mvol	324.860	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2424.00		NIST Webbook
rinpol	2424.00		NIST Webbook
tb	869.74	K	Joback Method
tc	1069.00	K	Joback Method
tf	462.92	K	Joback Method
vc	1.244	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.94	J/molxK	869.74	Joback Method
cpg	1105.16	J/molxK	902.95	Joback Method
cpg	1123.03	J/molxK	936.16	Joback Method
cpg	1139.59	J/molxK	969.37	Joback Method
cpg	1154.88	J/molxK	1002.58	Joback Method
cpg	1168.93	J/molxK	1035.79	Joback Method
cpg	1181.78	J/molxK	1069.00	Joback Method
dvisc	0.0011467	Paxs	462.92	Joback Method

dvisc	0.0004867	Paxs	530.72	Joback Method
dvisc	0.0002509	Paxs	598.53	Joback Method
dvisc	0.0001480	Paxs	666.33	Joback Method
dvisc	0.0000962	Paxs	734.13	Joback Method
dvisc	0.0000673	Paxs	801.94	Joback Method
dvisc	0.0000498	Paxs	869.74	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=U405467&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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