

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

Inchi:	InChI=1S/C19H34O4/c1-4-5-6-10-15(2)22-18(20)13-9-14-19(21)23-16(3)17-11-7-8-12-1
InchiKey:	JNSURHCIJYZVDW-UHFFFAOYSA-N
Formula:	C19H34O4
SMILES:	CCCCC(C)OC(=O)CCCC(=O)OC(C)C1CCCC1
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	-327.07	kJ/mol	Joback Method
hf	-875.17	kJ/mol	Joback Method
hfus	37.43	kJ/mol	Joback Method
hvap	75.68	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.791		Crippen Method
mvol	282.590	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	801.10	K	Joback Method
tc	996.43	K	Joback Method
tf	429.11	K	Joback Method
vc	1.077	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.59	J/molxK	801.10	Joback Method
cpg	921.36	J/molxK	833.66	Joback Method
cpg	938.92	J/molxK	866.21	Joback Method
cpg	955.30	J/molxK	898.77	Joback Method
cpg	970.52	J/molxK	931.32	Joback Method
cpg	984.62	J/molxK	963.88	Joback Method
cpg	997.61	J/molxK	996.43	Joback Method
dvisc	0.0016207	Paxs	429.11	Joback Method

dvisc	0.0007064	Paxs	491.11	Joback Method
dvisc	0.0003709	Paxs	553.11	Joback Method
dvisc	0.0002218	Paxs	615.11	Joback Method
dvisc	0.0001457	Paxs	677.10	Joback Method
dvisc	0.0001027	Paxs	739.10	Joback Method
dvisc	0.0000764	Paxs	801.10	Joback Method

Sources

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=U405463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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