

Glutaric acid, cyclopentyl hept-2-yl ester

Inchi:	InChI=1S/C17H30O4/c1-3-4-5-9-14(2)20-16(18)12-8-13-17(19)21-15-10-6-7-11-15/h14-1
InchiKey:	HSLUTSRUVLAMSU-UHFFFAOYSA-N
Formula:	C17H30O4
SMILES:	CCCCC(C)OC(=O)CCCC(=O)OC1CCCC1
Mol. weight [g/mol]:	298.42

Physical Properties

Property code	Value	Unit	Source
gf	-341.47	kJ/mol	Joback Method
hf	-828.61	kJ/mol	Joback Method
hfus	35.77	kJ/mol	Joback Method
hvap	71.62	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.155		Crippen Method
mcvol	254.410	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	755.78	K	Joback Method
tc	949.32	K	Joback Method
tf	421.57	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.75	J/molxK	755.78	Joback Method
cpg	864.05	J/molxK	917.06	Joback Method
cpg	850.11	J/molxK	884.81	Joback Method
cpg	835.13	J/molxK	852.55	Joback Method
cpg	819.09	J/molxK	820.29	Joback Method
cpg	801.97	J/molxK	788.04	Joback Method
cpg	876.97	J/molxK	949.32	Joback Method
dvisc	0.0001089	Paxs	755.78	Joback Method

dvisc	0.0001431	Paxs	700.08	Joback Method
dvisc	0.0001972	Paxs	644.38	Joback Method
dvisc	0.0002888	Paxs	588.67	Joback Method
dvisc	0.0004579	Paxs	532.97	Joback Method
dvisc	0.0008085	Paxs	477.27	Joback Method
dvisc	0.0016590	Paxs	421.57	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=U405392&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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