

Glutaric acid, cyclopentyl naphth-2-ylmethyl ester

Inchi:	InChI=1S/C21H24O4/c22-20(10-5-11-21(23)25-19-8-3-4-9-19)24-15-16-12-13-17-6-1-2-7
InchiKey:	YIGFCXDVEFLTQH-UHFFFAOYSA-N
Formula:	C21H24O4
SMILES:	O=C(CCCC(=O)OC1CCCC1)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	340.41

Physical Properties

Property code	Value	Unit	Source
gf	-95.92	kJ/mol	Joback Method
hf	-489.76	kJ/mol	Joback Method
hfus	40.33	kJ/mol	Joback Method
hvap	85.49	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.539		Crippen Method
mcvol	267.550	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	2882.00		NIST Webbook
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tb	898.38	K	Joback Method
tc	1128.85	K	Joback Method
tf	553.29	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.14	J/mol×K	898.38	Joback Method
cpg	915.34	J/mol×K	1090.44	Joback Method
cpg	904.75	J/mol×K	1052.02	Joback Method
cpg	893.11	J/mol×K	1013.61	Joback Method
cpg	880.35	J/mol×K	975.20	Joback Method
cpg	866.39	J/mol×K	936.79	Joback Method
cpg	924.96	J/mol×K	1128.85	Joback Method
dvisc	0.0001444	Pa×s	898.38	Joback Method

dvisc	0.0001763	Pa×s	840.87	Joback Method
dvisc	0.0002217	Pa×s	783.35	Joback Method
dvisc	0.0002889	Pa×s	725.84	Joback Method
dvisc	0.0003942	Pa×s	668.32	Joback Method
dvisc	0.0005701	Pa×s	610.80	Joback Method
dvisc	0.0008905	Pa×s	553.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405404&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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