

Glutaric acid, cyclohexylmethyl 2-hexyl ester

Inchi:	InChI=1S/C18H32O4/c1-3-4-9-15(2)22-18(20)13-8-12-17(19)21-14-16-10-6-5-7-11-16/h1
InchiKey:	FCRQWRSKRYOELY-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	CCCCC(C)OC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-345.15	kJ/mol	Joback Method
hf	-855.41	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.402		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	782.93	K	Joback Method
tc	980.01	K	Joback Method
tf	429.32	K	Joback Method
vc	1.018	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.45	J/molxK	782.93	Joback Method
cpg	865.30	J/molxK	815.78	Joback Method
cpg	882.92	J/molxK	848.62	Joback Method
cpg	899.31	J/molxK	881.47	Joback Method
cpg	914.51	J/molxK	914.31	Joback Method
cpg	928.52	J/molxK	947.16	Joback Method
cpg	941.36	J/molxK	980.01	Joback Method
dvisc	0.0014323	Paxs	429.32	Joback Method

dvisc	0.0006331	Paxs	488.25	Joback Method
dvisc	0.0003336	Paxs	547.19	Joback Method
dvisc	0.0001991	Paxs	606.12	Joback Method
dvisc	0.0001302	Paxs	665.06	Joback Method
dvisc	0.0000913	Paxs	723.99	Joback Method
dvisc	0.0000675	Paxs	782.93	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=U393601&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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