

Glutaric acid, cyclohexylmethyl 2-octyl ester

Inchi: InChI=1S/C20H36O4/c1-3-4-5-7-11-17(2)24-20(22)15-10-14-19(21)23-16-18-12-8-6-9-13
InchiKey: RXQQVMCAOFVZLC-UHFFFAOYSA-N
Formula: C20H36O4
SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-328.31	kJ/mol	Joback Method
hf	-896.69	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	78.47	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.182		Crippen Method
mvol	296.680	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	828.69	K	Joback Method
tc	1026.13	K	Joback Method
tf	451.86	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.84	J/molxK	828.69	Joback Method
cpg	985.88	J/molxK	861.60	Joback Method
cpg	1003.60	J/molxK	894.50	Joback Method
cpg	1020.03	J/molxK	927.41	Joback Method
cpg	1035.18	J/molxK	960.31	Joback Method
cpg	1049.09	J/molxK	993.22	Joback Method
cpg	1061.76	J/molxK	1026.13	Joback Method
dvisc	0.0011350	Paxs	451.86	Joback Method

dvisc	0.0004924	Paxs	514.66	Joback Method
dvisc	0.0002562	Paxs	577.47	Joback Method
dvisc	0.0001515	Paxs	640.27	Joback Method
dvisc	0.0000984	Paxs	703.08	Joback Method
dvisc	0.0000686	Paxs	765.88	Joback Method
dvisc	0.0000505	Paxs	828.69	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=U391451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

<https://www.chemeo.com/cid/87-738-7/Glutaric-acid-cyclohexylmethyl-2-octyl-ester.pdf>

Generated by Cheméo on 2024-04-25 09:25:23.801313502 +0000 UTC m=+16326372.721890823.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.