Glutaric acid, cyclohexylmethyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C20H36O4/c1-16(13-20(2,3)4)14-23-18(21)11-8-12-19(22)24-15-17-9-6-5-7-10

InchiKey: SOZSIQOAKKKNNY-UHFFFAOYSA-N

Formula: C20H36O4

SMILES: CC(COC(=O)CCCC(=O)OCC1CCCCC1)CC(C)(C)C

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-325.47	kJ/mol	Joback Method
hf	-905.44	kJ/mol	Joback Method
hfus	34.03	kJ/mol	Joback Method
hvap	77.17	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.896		Crippen Method
mcvol	296.680	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	2296.00		NIST Webbook
rinpol	2296.00		NIST Webbook
tb	825.46	K	Joback Method
tc	1028.06	K	Joback Method
tf	454.28	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.68	J/mol×K	825.46	Joback Method
cpg	1051.00	J/mol×K	994.29	Joback Method
cpg	1036.89	J/mol×K	960.53	Joback Method
cpg	1021.54	J/mol×K	926.76	Joback Method
cpg	1004.92	J/mol×K	892.99	Joback Method
cpg	986.98	J/mol×K	859.23	Joback Method
cpg	1063.92	J/mol×K	1028.06	Joback Method
dvisc	0.0000402	Pa×s	825.46	Joback Method

dvisc	0.0000558	Pa×s	763.60	Joback Method
dvisc	0.0000820	Pa×s	701.73	Joback Method
dvisc	0.0001297	Pa×s	639.87	Joback Method
dvisc	0.0002266	Pa×s	578.01	Joback Method
dvisc	0.0004522	Pa×s	516.14	Joback Method
dvisc	0.0010895	Pa×s	454.28	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=U391534&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