Glutaric acid, (2-methylcyclohex-1-enyl)methyl cyclohexylmethyl ester

Inchi: InChI=1S/C20H32O4/c1-16-8-5-6-11-18(16)15-24-20(22)13-7-12-19(21)23-14-17-9-3-2-4
InchiKey: FORLWRMUCYQMGW-UHFFFAOYSA-N
Formula: C20H32O4
SMILES: CC1=C(COC(=O)CCCC(=O)OCC2CCCCC2)CCCC1
Mol. weight [g/mol]: 336.47

Physical Properties

Property code	Value	Unit	Source
gf	-283.01	kJ/mol	Joback Method
hf	-781.91	kJ/mol	Joback Method
hfus	36.17	kJ/mol	Joback Method
hvap	81.21	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.714		Crippen Method
mcvol	281.520	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook
tb	862.47	K	Joback Method
tc	1079.46	K	Joback Method
tf	504.28	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.44	J/mol×K	862.47	Joback Method
cpg	948.89	J/mol×K	898.63	Joback Method
cpg	965.77	J/mol×K	934.80	Joback Method
cpg	981.09	J/mol×K	970.96	Joback Method
cpg	994.90	J/mol×K	1007.13	Joback Method
cpg	1007.21	J/mol×K	1043.29	Joback Method
cpg	1018.06	J/mol×K	1079.46	Joback Method
dvisc	0.0006927	Pa×s	504.28	Joback Method

dvisc	0.0003517	Pa×s	563.98	Joback Method
dvisc	0.0002034	Pa×s	623.68	Joback Method
dvisc	0.0001294	Pa×s	683.38	Joback Method
dvisc	0.0000885	Pa×s	743.07	Joback Method
dvisc	0.0000641	Pa×s	802.77	Joback Method
dvisc	0.0000485	Pa×s	862.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405507&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

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