Glutaric acid, cyclohexylmethyl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C20H28O5/c1-15-11-12-17(23-2)18(13-15)25-20(22)10-6-9-19(21)24-14-16-7-
InchiKey: FSWXPTCKQZFJTB-UHFFFAOYSA-N
Formula: C20H28O5
SMILES: COc1ccc(C)cc1OC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 348.43

Physical Properties

Property code	Value	Unit	Source
gf	-337.72	kJ/mol	Joback Method
hf	-810.04	kJ/mol	Joback Method
hfus	39.42	kJ/mol	Joback Method
hvap	84.86	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.203		Crippen Method
mcvol	278.790	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	888.19	K	Joback Method
tc	1107.78	K	Joback Method
tf	540.55	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.21	J/mol×K	888.19	Joback Method
cpg	917.21	J/mol×K	924.79	Joback Method
cpg	931.64	J/mol×K	961.39	Joback Method
cpg	944.49	J/mol×K	997.98	Joback Method
cpg	955.78	J/mol×K	1034.58	Joback Method
cpg	965.52	J/mol×K	1071.18	Joback Method
cpg	973.71	J/mol×K	1107.78	Joback Method
dvisc	0.0004094	Pa×s	540.55	Joback Method

dvisc	0.0002347	Pa×s	598.49	Joback Method
dvisc	0.0001484	Pa×s	656.43	Joback Method
dvisc	0.0001011	Pa×s	714.37	Joback Method
dvisc	0.0000729	Pa×s	772.31	Joback Method
dvisc	0.0000551	Pa×s	830.25	Joback Method
dvisc	0.0000431	Pa×s	888.19	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=U393928&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