Glutaric acid, hept-2-yl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C20H30O5/c1-5-6-7-9-16(3)24-19(21)10-8-11-20(22)25-18-14-15(2)12-13-17(1

InchiKey: JWMOCDZWUCOGJY-UHFFFAOYSA-N

Formula: C20H30O5

SMILES: CCCCCC(C)OC(=O)CCCC(=O)Oc1cc(C)ccc1OC

Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
gf	-364.61	kJ/mol	Joback Method
hf	-869.64	kJ/mol	Joback Method
hfus	44.06	kJ/mol	Joback Method
hvap	84.05	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.591		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
tb	868.20	K	Joback Method
tc	1072.07	K	Joback Method
tf	518.17	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.91	J/mol×K	868.20	Joback Method
cpg	922.55	J/mol×K	902.18	Joback Method
cpg	936.94	J/mol×K	936.16	Joback Method
cpg	950.09	J/mol×K	970.14	Joback Method
cpg	961.99	J/mol×K	1004.11	Joback Method
cpg	972.66	J/mol×K	1038.09	Joback Method
cpg	982.10	J/mol×K	1072.07	Joback Method
dvisc	0.0004006	Pa×s	518.17	Joback Method

dvisc	0.0002221	Pa×s	576.51	Joback Method
dvisc	0.0001372	Pa×s	634.85	Joback Method
dvisc	0.0000919	Pa×s	693.19	Joback Method
dvisc	0.0000655	Pa×s	751.52	Joback Method
dvisc	0.0000491	Pa×s	809.86	Joback Method
dvisc	0.0000382	Pa×s	868.20	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=U393925&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