Glutaric acid, hept-2-yl 4-chlorobenzyl ester

Inchi: InChI=1S/C19H27ClO4/c1-3-4-5-7-15(2)24-19(22)9-6-8-18(21)23-14-16-10-12-17(20)13-

InchiKey: ASHXZMQJXRAYIL-UHFFFAOYSA-N

Formula: C19H27ClO4

SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 354.87

Physical Properties

Property code	Value	Unit	Source
gf	-270.33	kJ/mol	Joback Method
hf	-721.05	kJ/mol	Joback Method
hfus	44.87	kJ/mol	Joback Method
hvap	83.14	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.065		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	2468.00		NIST Webbook
rinpol	2468.00		NIST Webbook
tb	855.35	K	Joback Method
tc	1061.57	K	Joback Method
tf	502.07	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.82	J/mol×K	855.35	Joback Method
cpg	861.69	J/mol×K	889.72	Joback Method
cpg	875.42	J/mol×K	924.09	Joback Method
cpg	888.04	J/mol×K	958.46	Joback Method
cpg	899.57	J/mol×K	992.83	Joback Method
cpg	910.03	J/mol×K	1027.20	Joback Method
cpg	919.45	J/mol×K	1061.57	Joback Method
dvisc	0.0006030	Pa×s	502.07	Joback Method

dvisc	0.0003202	Pa×s	560.95	Joback Method
dvisc	0.0001918	Pa×s	619.83	Joback Method
dvisc	0.0001256	Pa×s	678.71	Joback Method
dvisc	0.0000879	Pa×s	737.59	Joback Method
dvisc	0.0000649	Pa×s	796.47	Joback Method
dvisc	0.0000500	Pa×s	855.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391727&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