Glutaric acid, 8-chlorooctyl diphenylmethyl ester

Inchi: InChI=1S/C26H33ClO4/c27-20-11-3-1-2-4-12-21-30-24(28)18-13-19-25(29)31-26(22-14-
InchiKey: JALMUNBTROVTCA-UHFFFAOYSA-N
Formula: C26H33ClO4
SMILES: O=C(CCCC(=O)OC(c1ccccc1)c1ccccc1)OCCCCCCCCCCl
Mol. weight [g/mol]: 444.99

Physical Properties

Property code	Value	Unit	Source
gf	-89.35	kJ/mol	Joback Method
hf	-617.53	kJ/mol	Joback Method
hfus	57.43	kJ/mol	Joback Method
hvap	100.33	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.612		Crippen Method
mcvol	356.800	ml/mol	McGowan Method
pc	1119.30	kPa	Joback Method
rinpol	3351.00		NIST Webbook
rinpol	3351.00		NIST Webbook
tb	1037.21	K	Joback Method
tc	1271.01	K	Joback Method
tf	594.86	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.73	J/mol×K	1037.21	Joback Method
cpg	1175.15	J/mol×K	1076.18	Joback Method
cpg	1187.14	J/mol×K	1115.14	Joback Method
cpg	1197.76	J/mol×K	1154.11	Joback Method
cpg	1207.11	J/mol×K	1193.08	Joback Method
cpg	1215.25	J/mol×K	1232.05	Joback Method
cpg	1222.29	J/mol×K	1271.01	Joback Method
dvisc	0.0002617	Pa×s	594.86	Joback Method

dvisc	0.0001301	Pa×s	668.59	Joback Method
dvisc	0.0000743	Pa×s	742.31	Joback Method
dvisc	0.0000469	Pa×s	816.04	Joback Method
dvisc	0.0000320	Pa×s	889.76	Joback Method
dvisc	0.0000231	Pa×s	963.49	Joback Method
dvisc	0.0000175	Pa×s	1037.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393351&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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