Glutaric acid, 8-chlorooctyl 4-chlorobenzyl ester

Inchi: InChI=1S/C20H28Cl2O4/c21-14-5-3-1-2-4-6-15-25-19(23)8-7-9-20(24)26-16-17-10-12-18

InchiKey: XUGNKPYEOIYCCD-UHFFFAOYSA-N

Formula: C20H28Cl2O4

SMILES: O=C(CCCC(=O)OCc1ccc(Cl)cc1)OCCCCCCCCCCl

Mol. weight [g/mol]: 403.34

Physical Properties

Property code	Value	Unit	Source
gf	-271.40	kJ/mol	Joback Method
hf	-752.15	kJ/mol	Joback Method
hfus	55.18	kJ/mol	Joback Method
hvap	90.13	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.676		Crippen Method
mcvol	308.260	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	3049.00		NIST Webbook
rinpol	3049.00		NIST Webbook
tb	916.10	K	Joback Method
tc	1127.16	K	Joback Method
tf	558.26	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.17	J/mol×K	916.10	Joback Method
cpg	943.97	J/mol×K	951.28	Joback Method
cpg	956.60	J/mol×K	986.45	Joback Method
cpg	968.09	J/mol×K	1021.63	Joback Method
cpg	978.47	J/mol×K	1056.81	Joback Method
cpg	987.77	J/mol×K	1091.99	Joback Method
cpg	996.01	J/mol×K	1127.16	Joback Method
dvisc	0.0003923	Pa×s	558.26	Joback Method

dvisc	0.0002234	Pa×s	617.90	Joback Method
dvisc	0.0001405	Pa×s	677.54	Joback Method
dvisc	0.0000953	Pa×s	737.18	Joback Method
dvisc	0.0000685	Pa×s	796.82	Joback Method
dvisc	0.0000515	Pa×s	856.46	Joback Method
dvisc	0.0000402	Pa×s	916.10	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=U391734&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