Glutaric acid, 2,2-dichloroethyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C20H20Cl2O5/c21-18(22)14-26-20(24)11-5-10-19(23)25-13-15-6-4-9-17(12-15
InchiKey: NXHURRGYZYMSAY-UHFFFAOYSA-N
Formula: C20H20Cl2O5
SMILES: O=C(CCCC(=O)OCC(Cl)Cl)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 411.28

Physical Properties

Property code	Value	Unit	Source
gf	-266.43	kJ/mol	Joback Method
hf	-653.12	kJ/mol	Joback Method
hfus	46.88	kJ/mol	Joback Method
hvap	94.43	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.039		Crippen Method
mcvol	290.370	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	3002.00		NIST Webbook
rinpol	3002.00		NIST Webbook
tb	964.76	K	Joback Method
tc	1198.09	K	Joback Method
tf	591.91	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.00	J/mol×K	964.76	Joback Method
cpg	862.61	J/mol×K	1003.65	Joback Method
cpg	871.80	J/mol×K	1042.54	Joback Method
cpg	879.60	J/mol×K	1081.42	Joback Method
cpg	886.05	J/mol×K	1120.31	Joback Method
cpg	891.18	J/mol×K	1159.20	Joback Method
cpg	895.01	J/mol×K	1198.09	Joback Method
dvisc	0.0002657	Pa×s	591.91	Joback Method

dvisc	0.0001528	Pa×s	654.05	Joback Method
dvisc	0.0000967	Pa×s	716.19	Joback Method
dvisc	0.0000658	Pa×s	778.34	Joback Method
dvisc	0.0000474	Pa×s	840.48	Joback Method
dvisc	0.0000358	Pa×s	902.62	Joback Method
dvisc	0.0000280	Pa×s	964.76	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=U392125&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