Glutaric acid, 2,4,6-trichlorophenyl pentafluorophenyl ester

Inchi: InChI=1S/C17H8Cl3F5O4/c18-6-4-7(19)16(8(20)5-6)28-9(26)2-1-3-10(27)29-17-14(24)12
InchiKey: BJDNDTYCXGRKOX-UHFFFAOYSA-N
Formula: C17H8Cl3F5O4
SMILES: O=C(CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 477.59

Physical Properties

Property code	Value	Unit	Source
gf	-1237.64	kJ/mol	Joback Method
hf	-1530.28	kJ/mol	Joback Method
hfus	58.32	kJ/mol	Joback Method
hvap	90.67	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.024		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	942.78	K	Joback Method
tc	1161.15	K	Joback Method
tf	671.38	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.12	J/mol×K	942.78	Joback Method
cpg	706.47	J/mol×K	979.18	Joback Method
cpg	712.77	J/mol×K	1015.57	Joback Method
cpg	718.00	J/mol×K	1051.97	Joback Method
cpg	722.16	J/mol×K	1088.36	Joback Method
cpg	725.24	J/mol×K	1124.76	Joback Method
cpg	727.23	J/mol×K	1161.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392116&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
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