Glutaric acid, 2,3-dichlorophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C18H11Cl2F5O4/c19-9-3-1-4-10(13(9)20)29-12(27)6-2-5-11(26)28-7-8-14(21)1

InchiKey: QKJKMMQWMZNQBV-UHFFFAOYSA-N

Formula: C18H11Cl2F5O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 457.18

Physical Properties

Property code	Value	Unit	Source
gf	-1207.66	kJ/mol	Joback Method
hf	-1523.71	kJ/mol	Joback Method
hfus	57.10	kJ/mol	Joback Method
hvap	87.84	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	5.508		Crippen Method
mcvol	265.170	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	923.25	K	Joback Method
tc	1136.66	K	Joback Method
tf	640.21	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.76	J/mol×K	923.25	Joback Method
cpg	747.62	J/mol×K	958.82	Joback Method
cpg	755.43	J/mol×K	994.39	Joback Method
cpg	762.18	J/mol×K	1029.95	Joback Method
cpg	767.87	J/mol×K	1065.52	Joback Method
cpg	772.50	J/mol×K	1101.09	Joback Method
cpg	776.08	J/mol×K	1136.66	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=U391940&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
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