Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C17H12F12O4/c18-12-8(16(25,26)27)3-1-4-9(12)33-11(31)6-2-5-10(30)32-7-1

InchiKey: JGLYBJYDMMQZJZ-UHFFFAOYSA-N

Formula: C17H12F12O4

SMILES: O=C(CCCC(=O)Oc1cccc(C(F)(F)F)c1F)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 508.26

Physical Properties

Property code	Value	Unit	Source
gf	-2611.23	kJ/mol	Joback Method
hf	-3063.82	kJ/mol	Joback Method
hfus	42.40	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.634		Crippen Method
mcvol	262.750	ml/mol	McGowan Method
pc	1178.47	kPa	Joback Method
rinpol	1792.00		NIST Webbook
rinpol	1792.00		NIST Webbook
tb	755.46	K	Joback Method
tc	928.14	K	Joback Method
tf	478.89	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.40	J/mol×K	755.46	Joback Method
cpg	815.72	J/mol×K	784.24	Joback Method
cpg	826.21	J/mol×K	813.02	Joback Method
cpg	835.93	J/mol×K	841.80	Joback Method
cpg	844.93	J/mol×K	870.58	Joback Method
cpg	853.27	J/mol×K	899.36	Joback Method
cpg	861.01	J/mol×K	928.14	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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