Glutaric acid, 2-fluorophenyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C15H13F7O4/c16-9-4-1-2-5-10(9)26-12(24)7-3-6-11(23)25-8-14(18,19)13(17)1

InchiKey: DOQLZDCHDSRDQW-UHFFFAOYSA-N

Formula: C15H13F7O4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCC(F)(F)C(F)C(F)(F)F

Mol. weight [g/mol]: 390.25

Physical Properties

Property code	Value	Unit	Source
gf	-1650.07	kJ/mol	Joback Method
hf	-2013.02	kJ/mol	Joback Method
hfus	37.04	kJ/mol	Joback Method
hvap	61.53	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.980		Crippen Method
mcvol	225.720	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	714.83	K	Joback Method
tc	893.18	K	Joback Method
tf	436.04	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.06	J/mol×K	714.83	Joback Method
cpg	666.10	J/mol×K	744.56	Joback Method
cpg	677.33	J/mol×K	774.28	Joback Method
cpg	687.77	J/mol×K	804.01	Joback Method
cpg	697.47	J/mol×K	833.73	Joback Method
cpg	706.46	J/mol×K	863.46	Joback Method
cpg	714.78	J/mol×K	893.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393689&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

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