Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C15H13F7O4/c1-8(14(17,18)19)25-11(23)6-3-7-12(24)26-10-5-2-4-9(13(10)16)

InchiKey: UGQJIHJACJGPBP-UHFFFAOYSA-N

Formula: C15H13F7O4

SMILES: CC(OC(=O)CCCC(=O)Oc1cccc(C(F)(F)F)c1F)C(F)(F)F

Mol. weight [g/mol]: 390.25

Physical Properties

Property code	Value	Unit	Source
gf	-1659.70	kJ/mol	Joback Method
hf	-2024.49	kJ/mol	Joback Method
hfus	36.65	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.414		Crippen Method
mcvol	225.720	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	719.81	K	Joback Method
tc	899.03	K	Joback Method
tf	448.56	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.07	J/mol×K	719.81	Joback Method
cpg	664.99	J/mol×K	749.68	Joback Method
cpg	676.11	J/mol×K	779.55	Joback Method
cpg	686.46	J/mol×K	809.42	Joback Method
cpg	696.09	J/mol×K	839.29	Joback Method
cpg	705.00	J/mol×K	869.16	Joback Method
cpg	713.25	J/mol×K	899.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393611&Units=SI

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