Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C16H11F11O4/c17-7-4-5-8(12(19)11(7)18)31-10(29)3-1-2-9(28)30-6-14(22,23

InchiKey: DZCZUVZIGXUXOT-UHFFFAOYSA-N

Formula: C16H11F11O4

SMILES: O=C(CCCC(=O)Oc1ccc(F)c(F)c1F)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 476.24

Physical Properties

Property code	Value	Unit	Source
gf	-2437.31	kJ/mol	Joback Method
hf	-2849.79	kJ/mol	Joback Method
hfus	43.76	kJ/mol	Joback Method
hvap	60.52	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	4.894		Crippen Method
mcvol	246.890	ml/mol	McGowan Method
pc	1270.06	kPa	Joback Method
rinpol	1794.00		NIST Webbook
rinpol	1794.00		NIST Webbook
tb	741.52	K	Joback Method
tc	912.56	K	Joback Method
tf	477.13	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.25	J/mol×K	741.52	Joback Method
cpg	750.32	J/mol×K	770.03	Joback Method
cpg	760.61	J/mol×K	798.53	Joback Method
cpg	770.19	J/mol×K	827.04	Joback Method
cpg	779.07	J/mol×K	855.55	Joback Method
cpg	787.30	J/mol×K	884.06	Joback Method
cpg	794.92	J/mol×K	912.56	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=U393634&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