Glutaric acid, 2,2,3,3-tetrafluoropropyl 2-formylphenyl ester

Inchi: InChI=1S/C15H14F4O5/c16-14(17)15(18,19)9-23-12(21)6-3-7-13(22)24-11-5-2-1-4-10(1

InchiKey: OHEDQDZEASKTMT-UHFFFAOYSA-N

Formula: C15H14F4O5

SMILES: O=Cc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 350.26

Physical Properties

Property code	Value	Unit	Source
gf	-1168.00	kJ/mol	Joback Method
hf	-1501.52	kJ/mol	Joback Method
hfus	37.50	kJ/mol	Joback Method
hvap	72.00	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.018		Crippen Method
mcvol	221.980	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	2031.00		NIST Webbook
rinpol	2031.00		NIST Webbook
tb	768.91	K	Joback Method
tc	961.41	K	Joback Method
tf	473.85	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.92	J/mol×K	768.91	Joback Method
cpg	654.42	J/mol×K	800.99	Joback Method
cpg	665.07	J/mol×K	833.08	Joback Method
cpg	674.89	J/mol×K	865.16	Joback Method
cpg	683.91	J/mol×K	897.24	Joback Method
cpg	692.16	J/mol×K	929.32	Joback Method
cpg	699.66	J/mol×K	961.41	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=U390488&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