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

Inchi: InChI=1S/C15H11F9O4/c16-9-6(10(17)12(19)13(20)11(9)18)4-27-7(25)2-1-3-8(26)28-5-1

InchiKey: RDLRXAYEINDPIQ-UHFFFAOYSA-N

Formula: C15H11F9O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)F)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 426.23

Physical Properties

Property code	Value	Unit	Source
gf	-2081.05	kJ/mol	Joback Method
hf	-2442.37	kJ/mol	Joback Method
hfus	49.06	kJ/mol	Joback Method
hvap	63.84	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.039		Crippen Method
mcvol	229.260	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	736.52	K	Joback Method
tc	907.09	K	Joback Method
tf	484.88	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.04	J/mol×K	736.52	Joback Method
cpg	674.00	J/mol×K	764.95	Joback Method
cpg	684.30	J/mol×K	793.38	Joback Method
cpg	693.95	J/mol×K	821.80	Joback Method
cpg	702.96	J/mol×K	850.23	Joback Method
cpg	711.33	J/mol×K	878.66	Joback Method
cpg	719.08	J/mol×K	907.09	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=U391925&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