Glutaric acid, di(2-(pentafluorophenoxy)ethyl) ester

Inchi: InChI=1S/C21H14F10O6/c22-10-12(24)16(28)20(17(29)13(10)25)36-6-4-34-8(32)2-1-3-9

InchiKey: XESNITKCYHAJGC-UHFFFAOYSA-N

Formula: C21H14F10O6

SMILES: O=C(CCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F)OCCOc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 552.32

Physical Properties

Property code	Value	Unit	Source
gf	-2371.48	kJ/mol	Joback Method
hf	-2833.55	kJ/mol	Joback Method
hfus	73.09	kJ/mol	Joback Method
hvap	88.47	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	4.792		Crippen Method
mcvol	303.550	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	2617.00		NIST Webbook
tb	973.16	K	Joback Method
tc	1199.82	K	Joback Method
tf	699.15	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.96	J/mol×K	973.16	Joback Method
cpg	960.66	J/mol×K	1010.94	Joback Method
cpg	968.59	J/mol×K	1048.71	Joback Method
cpg	974.70	J/mol×K	1086.49	Joback Method
cpg	978.96	J/mol×K	1124.26	Joback Method
cpg	981.32	J/mol×K	1162.04	Joback Method
cpg	981.72	J/mol×K	1199.82	Joback Method

Sources

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=U377332&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/48-367-2/Glutaric-acid-di-2-pentafluorophenoxy-ethyl-ester.pdf
Generated by Cheméo on 2024-04-29 22:37:00.438823291 +0000 UTC m=+16719469.359400606.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.