Glutaric acid, 2-methylhex-3-yl 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C20H25F5O5/c1-4-6-12(11(2)3)30-14(27)8-5-7-13(26)28-9-10-29-20-18(24)16
InchiKey: VLEWIYLGDUSBDZ-UHFFFAOYSA-N
Formula: C20H25F5O5
SMILES: CCCC(OC(=O)CCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 440.40

Physical Properties

Property code	Value	Unit	Source
gf	-1369.99	kJ/mol	Joback Method
hf	-1889.88	kJ/mol	Joback Method
hfus	54.77	kJ/mol	Joback Method
hvap	81.56	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	4.842		Crippen Method
mcvol	298.500	ml/mol	McGowan Method
pc	1099.35	kPa	Joback Method
rinpol	2316.00		NIST Webbook
rinpol	2316.00		NIST Webbook
tb	879.05	K	Joback Method
tc	1076.28	K	Joback Method
tf	543.68	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.34	J/mol×K	879.05	Joback Method
cpg	955.46	J/mol×K	911.92	Joback Method
cpg	968.39	J/mol×K	944.79	Joback Method
cpg	980.11	J/mol×K	977.66	Joback Method
cpg	990.62	J/mol×K	1010.53	Joback Method
cpg	999.92	J/mol×K	1043.40	Joback Method
cpg	1008.00	J/mol×K	1076.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377325&Units=SI
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

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