Fumaric acid, pentafluorophenyl undecyl ester

Inchi: InChI=1S/C21H25F5O4/c1-2-3-4-5-6-7-8-9-10-13-29-14(27)11-12-15(28)30-21-19(25)17
InchiKey: FGACRZJSNKXPOP-VAWYXSNFSA-N
Formula: C21H25F5O4
SMILES: CCCCCCCCCCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 436.41

Physical Properties

Property code	Value	Unit	Source
gf	-1171.47	kJ/mol	Joback Method
hf	-1650.52	kJ/mol	Joback Method
hfus	63.42	kJ/mol	Joback Method
hvap	82.11	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	5.918		Crippen Method
mcvol	302.420	ml/mol	McGowan Method
pc	1068.66	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	884.55	K	Joback Method
tc	1082.95	K	Joback Method
tf	557.64	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.40	J/mol×K	884.55	Joback Method
cpg	957.71	J/mol×K	917.62	Joback Method
cpg	970.96	J/mol×K	950.68	Joback Method
cpg	983.18	J/mol×K	983.75	Joback Method
cpg	994.40	J/mol×K	1016.81	Joback Method
cpg	1004.61	J/mol×K	1049.88	Joback Method
cpg	1013.86	J/mol×K	1082.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348103&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