Fumaric acid, decyl pentafluorophenyl ester

Inchi: InChI=1S/C20H23F5O4/c1-2-3-4-5-6-7-8-9-12-28-13(26)10-11-14(27)29-20-18(24)16(22
InchiKey: XAAGOJQKXUUGDQ-ZHACJKMWSA-N
Formula: C20H23F5O4
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 422.39

Physical Properties

Property code	Value	Unit	Source
gf	-1179.89	kJ/mol	Joback Method
hf	-1629.88	kJ/mol	Joback Method
hfus	60.83	kJ/mol	Joback Method
hvap	79.89	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	5.528		Crippen Method
mcvol	288.330	ml/mol	McGowan Method
pc	1139.03	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	861.67	K	Joback Method
tc	1055.53	K	Joback Method
tf	546.37	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.71	J/mol×K	861.67	Joback Method
cpg	898.54	J/mol×K	893.98	Joback Method
cpg	911.41	J/mol×K	926.29	Joback Method
cpg	923.33	J/mol×K	958.60	Joback Method
cpg	934.31	J/mol×K	990.91	Joback Method
cpg	944.36	J/mol×K	1023.22	Joback Method
cpg	953.51	J/mol×K	1055.53	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348102&Units=SI

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