Fumaric acid, pentafluorobenzyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C22H13F5O4/c23-18-15(19(24)21(26)22(27)20(18)25)11-31-17(29)8-7-16(28)
InchiKey: GMUUXZYTMUABJY-BQYQJAHWSA-N
Formula: C22H13F5O4
SMILES: O=C(C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F)OCc1ccc2ccccc2c1
Mol. weight [g/mol]: 436.33

Physical Properties

Property code	Value	Unit	Source
gf	-953.62	kJ/mol	Joback Method
hf	-1255.03	kJ/mol	Joback Method
hfus	56.68	kJ/mol	Joback Method
hvap	88.92	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	4.878		Crippen Method
mcvol	273.290	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	2846.00		NIST Webbook
rinpol	2846.00		NIST Webbook
tb	958.07	K	Joback Method
tc	1179.57	K	Joback Method
tf	640.55	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.46	J/mol×K	958.07	Joback Method
cpg	826.74	J/mol×K	994.99	Joback Method
cpg	836.10	J/mol×K	1031.90	Joback Method
cpg	844.60	J/mol×K	1068.82	Joback Method
cpg	852.30	J/mol×K	1105.73	Joback Method
cpg	859.24	J/mol×K	1142.65	Joback Method
cpg	865.48	J/mol×K	1179.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405888&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