Fumaric acid, naphth-2-yl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C19H12F8O4/c20-16(21)18(24,25)19(26,27)17(22,23)10-30-14(28)7-8-15(29)3

InchiKey: FIUMQLALCJHFDF-BQYQJAHWSA-N

Formula: C19H12F8O4

SMILES: O=C(C=CC(=O)Oc1ccc2ccccc2c1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 456.28

Physical Properties

Property code	Value	Unit	Source
gf	-1621.49	kJ/mol	Joback Method
hf	-1992.15	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hvap	69.92	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.016		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	2307.00		NIST Webbook
rinpol	2307.00		NIST Webbook
tb	825.53	K	Joback Method
tc	1023.88	K	Joback Method
tf	511.75	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.81	J/mol×K	825.53	Joback Method
cpg	794.60	J/mol×K	858.59	Joback Method
cpg	804.60	J/mol×K	891.65	Joback Method
cpg	813.92	J/mol×K	924.70	Joback Method
cpg	822.67	J/mol×K	957.76	Joback Method
cpg	830.94	J/mol×K	990.82	Joback Method
cpg	838.85	J/mol×K	1023.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405823&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