Fumaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl undecyl ester

Inchi: InChI=1S/C20H28F8O4/c1-2-3-4-5-6-7-8-9-10-13-31-15(29)11-12-16(30)32-14-18(23,24

InchiKey: YUSCWXMPPJBOBL-VAWYXSNFSA-N

Formula: C20H28F8O4

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

Mol. weight [g/mol]: 484.42

Physical Properties

Property code	Value	Unit	Source
gf	-1822.50	kJ/mol	Joback Method
hf	-2428.92	kJ/mol	Joback Method
hfus	52.21	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.331		Crippen Method
mcvol	317.400	ml/mol	McGowan Method
pc	924.43	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	797.77	K	Joback Method
tc	976.69	K	Joback Method
tf	451.38	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1007.53	J/mol×K	797.77	Joback Method
cpg	1023.16	J/mol×K	827.59	Joback Method
cpg	1037.85	J/mol×K	857.41	Joback Method
cpg	1051.67	J/mol×K	887.23	Joback Method
cpg	1064.67	J/mol×K	917.05	Joback Method
cpg	1076.92	J/mol×K	946.87	Joback Method
cpg	1088.50	J/mol×K	976.69	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=U348787&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