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

Inchi: InChI=1S/C23H34F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-34-18(32)14-15-19(33)35-17

InchiKey: ZIPBMKNEKKDDTJ-CCEZHUSRSA-N

Formula: C23H34F8O4

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

Mol. weight [g/mol]: 526.50

Physical Properties

Property code	Value	Unit	Source
gf	-1797.24	kJ/mol	Joback Method
hf	-2490.84	kJ/mol	Joback Method
hfus	59.98	kJ/mol	Joback Method
hvap	74.25	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.501		Crippen Method
mcvol	359.670	ml/mol	McGowan Method
pc	781.56	kPa	Joback Method
rinpol	2416.00		NIST Webbook
rinpol	2416.00		NIST Webbook
tb	866.41	K	Joback Method
tc	1064.95	K	Joback Method
tf	485.19	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.02	J/mol×K	866.41	Joback Method
cpg	1204.68	J/mol×K	899.50	Joback Method
cpg	1221.22	J/mol×K	932.59	Joback Method
cpg	1236.75	J/mol×K	965.68	Joback Method
cpg	1251.36	J/mol×K	998.77	Joback Method
cpg	1265.14	J/mol×K	1031.86	Joback Method
cpg	1278.19	J/mol×K	1064.95	Joback Method

Sources

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=U348790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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