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

Inchi: InChI=1S/C28H44F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-39-23(37)19
InchiKey: QQVITBKEIHTHPR-FMQUCBEESA-N
Formula: C28H44F8O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 596.63

Physical Properties

Property code	Value	Unit	Source
gf	-1755.14	kJ/mol	Joback Method
hf	-2594.04	kJ/mol	Joback Method
hfus	72.93	kJ/mol	Joback Method
hvap	85.38	kJ/mol	Joback Method
log10ws	-10.38		Crippen Method
logp	9.452		Crippen Method
mcvol	430.120	ml/mol	McGowan Method
pc	607.56	kPa	Joback Method
rinpol	2878.00		NIST Webbook
rinpol	2878.00		NIST Webbook
tb	980.81	K	Joback Method
tc	1235.46	K	Joback Method
tf	541.54	K	Joback Method
vc	1.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1499.36	J/mol×K	980.81	Joback Method
cpg	1522.08	J/mol×K	1023.25	Joback Method
cpg	1543.24	J/mol×K	1065.69	Joback Method
cpg	1563.07	J/mol×K	1108.13	Joback Method
cpg	1581.80	J/mol×K	1150.57	Joback Method
cpg	1599.66	J/mol×K	1193.02	Joback Method
cpg	1616.88	J/mol×K	1235.46	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=U348795&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