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

Inchi: InChI=1S/C19H26F8O4/c1-2-3-4-5-6-7-8-9-12-30-14(28)10-11-15(29)31-13-17(22,23)19

InchiKey: RABMQDXGVSIRLK-ZHACJKMWSA-N

Formula: C19H26F8O4

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

Mol. weight [g/mol]: 470.39

Physical Properties

Property code	Value	Unit	Source
gf	-1830.92	kJ/mol	Joback Method
hf	-2408.28	kJ/mol	Joback Method
hfus	49.62	kJ/mol	Joback Method
hvap	65.35	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.941		Crippen Method
mcvol	303.310	ml/mol	McGowan Method
pc	980.85	kPa	Joback Method
rinpol	2044.00		NIST Webbook
rinpol	2044.00		NIST Webbook
tb	774.89	K	Joback Method
tc	949.09	K	Joback Method
tf	440.11	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.28	J/mol×K	774.89	Joback Method
cpg	964.34	J/mol×K	803.92	Joback Method
cpg	978.51	J/mol×K	832.96	Joback Method
cpg	991.85	J/mol×K	861.99	Joback Method
cpg	1004.39	J/mol×K	891.02	Joback Method
cpg	1016.22	J/mol×K	920.06	Joback Method
cpg	1027.38	J/mol×K	949.09	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=U348786&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