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

Inchi: InChI=1S/C29H46F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-40-24(38

InchiKey: LZGRDDZNNSUUJU-QZQOTICOSA-N

Formula: C29H46F8O4

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

Mol. weight [g/mol]: 610.66

Physical Properties

Property code	Value	Unit	Source
gf	-1746.72	kJ/mol	Joback Method
hf	-2614.68	kJ/mol	Joback Method
hfus	75.52	kJ/mol	Joback Method
hvap	87.61	kJ/mol	Joback Method
log10ws	-10.80		Crippen Method
logp	9.842		Crippen Method
mcvol	444.210	ml/mol	McGowan Method
pc	579.80	kPa	Joback Method
rinpol	2994.00		NIST Webbook
tb	1003.69	K	Joback Method
tc	1274.03	K	Joback Method
tf	552.81	K	Joback Method
vc	1.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1563.49	J/mol×K	1003.69	Joback Method
cpg	1587.58	J/mol×K	1048.75	Joback Method
cpg	1610.00	J/mol×K	1093.80	Joback Method
cpg	1631.03	J/mol×K	1138.86	Joback Method
cpg	1650.95	J/mol×K	1183.92	Joback Method
cpg	1670.05	J/mol×K	1228.98	Joback Method
cpg	1688.60	J/mol×K	1274.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348796&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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