

Isophthalic acid, octadecyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi:	InChI=1S/C31H44F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-42-26(40)24-19
InchiKey:	HDARURHOIFEKFC-UHFFFAOYSA-N
Formula:	C31H44F8O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)c1
Mol. weight [g/mol]:	632.67

Physical Properties

Property code	Value	Unit	Source
gf	-1707.32	kJ/mol	Joback Method
hf	-2548.12	kJ/mol	Joback Method
hfus	74.15	kJ/mol	Joback Method
hvap	95.04	kJ/mol	Joback Method
log10ws	-12.00		Crippen Method
logp	10.433		Crippen Method
mvol	452.930	ml/mol	McGowan Method
pc	600.44	kPa	Joback Method
rinpol	3267.00		NIST Webbook
rinpol	3267.00		NIST Webbook
tb	1076.95	K	Joback Method
tc	1365.74	K	Joback Method
tf	619.37	K	Joback Method
vc	1.817	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1612.43	J/mol×K	1076.95	Joback Method
cpg	1634.01	J/mol×K	1125.08	Joback Method
cpg	1653.92	J/mol×K	1173.21	Joback Method
cpg	1672.48	J/mol×K	1221.34	Joback Method
cpg	1690.03	J/mol×K	1269.47	Joback Method
cpg	1706.88	J/mol×K	1317.61	Joback Method
cpg	1723.38	J/mol×K	1365.74	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=U356602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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