

Phthalic acid, 2,2,3,3,4,4,4-heptafluorobutyl octadecyl ester

Inchi:	InChI=1S/C30H43F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-40-26(38)24-20
InchiKey:	SZISVCLFFYVJMY-UHFFFAOYSA-N
Formula:	C30H43F7O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1cccc1C(=O)OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	600.65

Physical Properties

Property code	Value	Unit	Source
gf	-1518.49	kJ/mol	Joback Method
hf	-2326.09	kJ/mol	Joback Method
hfus	72.00	kJ/mol	Joback Method
hvap	94.02	kJ/mol	Joback Method
log10ws	-11.62		Crippen Method
logp	10.095		Crippen Method
mvol	437.070	ml/mol	McGowan Method
pc	641.57	kPa	Joback Method
rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
tb	1055.24	K	Joback Method
tc	1323.95	K	Joback Method
tf	622.51	K	Joback Method
vc	1.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1542.06	J/molxK	1055.24	Joback Method
cpg	1562.45	J/molxK	1100.03	Joback Method
cpg	1581.31	J/molxK	1144.81	Joback Method
cpg	1598.90	J/molxK	1189.60	Joback Method
cpg	1615.48	J/molxK	1234.38	Joback Method
cpg	1631.30	J/molxK	1279.17	Joback Method
cpg	1646.62	J/molxK	1323.95	Joback Method

Sources

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=U415555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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