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

Inchi: InChI=1S/C21H25F7O4/c1-2-3-4-5-6-7-10-13-31-17(29)15-11-8-9-12-16(15)18(30)32-14

InchiKey: AKMOKMVKYVLVJA-UHFFFAOYSA-N

Formula: C21H25F7O4

SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 474.41

Physical Properties

Property code	Value	Unit	Source
gf	-1594.27	kJ/mol	Joback Method
hf	-2140.33	kJ/mol	Joback Method
hfus	48.69	kJ/mol	Joback Method
hvap	73.98	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	6.584		Crippen Method
mcvol	310.260	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2221.00		NIST Webbook
rinpol	2221.00		NIST Webbook
tb	849.32	K	Joback Method
tc	1040.91	K	Joback Method
tf	521.08	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	991.02	J/mol×K	849.32	Joback Method
cpg	1005.26	J/mol×K	881.25	Joback Method
cpg	1018.51	J/mol×K	913.18	Joback Method
cpg	1030.85	J/mol×K	945.12	Joback Method
cpg	1042.33	J/mol×K	977.05	Joback Method
cpg	1053.05	J/mol×K	1008.98	Joback Method
cpg	1063.06	J/mol×K	1040.91	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=U415547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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