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

Inchi: InChI=1S/C29H41F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-39-25(37)23-19-16

InchiKey: HVQOSRTYUVITIV-UHFFFAOYSA-N

Formula: C29H41F7O4

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

Mol. weight [g/mol]: 586.62

Physical Properties

Property code	Value	Unit	Source
gf	-1526.91	kJ/mol	Joback Method
hf	-2305.45	kJ/mol	Joback Method
hfus	69.41	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-11.20		Crippen Method
logp	9.704		Crippen Method
mcvol	422.980	ml/mol	McGowan Method
pc	673.95	kPa	Joback Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook
tb	1032.36	K	Joback Method
tc	1287.24	K	Joback Method
tf	611.24	K	Joback Method
vc	1.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1478.69	J/mol×K	1032.36	Joback Method
cpg	1498.05	J/mol×K	1074.84	Joback Method
cpg	1515.97	J/mol×K	1117.32	Joback Method
cpg	1532.67	J/mol×K	1159.80	Joback Method
cpg	1548.34	J/mol×K	1202.28	Joback Method
cpg	1563.20	J/mol×K	1244.76	Joback Method
cpg	1577.47	J/mol×K	1287.24	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=U415554&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