1,2-Cyclohexanedicarboxylic acid, pentadecyl pentafluorobenzyl ester

Inchi: InChI=1S/C30H43F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-19-38-29(36)21-17-14-15-18

InchiKey: CUZCJQVRFTZJRG-UHFFFAOYSA-N

Formula: C30H43F5O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 562.65

Physical Properties

Property code	Value	Unit	Source
gf	-1159.17	kJ/mol	Joback Method
hf	-1919.52	kJ/mol	Joback Method
hfus	79.43	kJ/mol	Joback Method
hvap	102.31	kJ/mol	Joback Method
log10ws	-10.77		Crippen Method
logp	8.866		Crippen Method
mcvol	422.670	ml/mol	McGowan Method
pc	691.43	kPa	Joback Method
tb	1101.19	K	Joback Method
tc	1376.83	K	Joback Method
tf	667.29	K	Joback Method
vc	1.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.41	J/mol×K	1101.19	Joback Method
cpg	1537.30	J/mol×K	1147.13	Joback Method
cpg	1550.20	J/mol×K	1193.07	Joback Method
cpg	1560.17	J/mol×K	1239.01	Joback Method
cpg	1567.30	J/mol×K	1284.95	Joback Method
cpg	1571.65	J/mol×K	1330.89	Joback Method
cpg	1573.30	J/mol×K	1376.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339826&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume