1,2-Cyclohexanedicarboxylic acid, pentafluorobenzyl tetradecyl ester

Inchi: InChI=1S/C29H41F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-37-28(35)20-16-13-14-17-21

InchiKey: SNYIBGQVLPRLLZ-UHFFFAOYSA-N

Formula: C29H41F5O4

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

Mol. weight [g/mol]: 548.63

Physical Properties

Property code	Value	Unit	Source
gf	-1167.59	kJ/mol	Joback Method
hf	-1898.88	kJ/mol	Joback Method
hfus	76.84	kJ/mol	Joback Method
hvap	100.08	kJ/mol	Joback Method
log10ws	-10.35		Crippen Method
logp	8.476		Crippen Method
mcvol	408.580	ml/mol	McGowan Method
pc	727.70	kPa	Joback Method
rinpol	3169.00		NIST Webbook
rinpol	3169.00		NIST Webbook
tb	1078.31	K	Joback Method
tc	1340.56	K	Joback Method
tf	656.02	K	Joback Method
vc	1.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1459.15	J/mol×K	1078.31	Joback Method
cpg	1474.98	J/mol×K	1122.02	Joback Method
cpg	1488.12	J/mol×K	1165.73	Joback Method
cpg	1498.61	J/mol×K	1209.43	Joback Method
cpg	1506.53	J/mol×K	1253.14	Joback Method
cpg	1511.93	J/mol×K	1296.85	Joback Method
cpg	1514.87	J/mol×K	1340.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339825&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume