Adipic acid, butyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C15H20F8O4/c1-2-3-8-26-10(24)6-4-5-7-11(25)27-9-13(18,19)15(22,23)14(20

InchiKey: SGVBBUGPAYSVHM-UHFFFAOYSA-N

Formula: C15H20F8O4

SMILES: CCCCOC(=O)CCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 416.30

Physical Properties

Property code	Value	Unit	Source
gf	-1944.82	kJ/mol	Joback Method
hf	-2442.94	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	56.48	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.604		Crippen Method
mcvol	251.250	ml/mol	McGowan Method
pc	1221.70	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
tb	679.21	K	Joback Method
tc	838.50	K	Joback Method
tf	400.11	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.96	J/mol×K	679.21	Joback Method
cpg	761.69	J/mol×K	705.76	Joback Method
cpg	774.65	J/mol×K	732.31	Joback Method
cpg	786.87	J/mol×K	758.85	Joback Method
cpg	798.39	J/mol×K	785.40	Joback Method
cpg	809.24	J/mol×K	811.95	Joback Method
cpg	819.44	J/mol×K	838.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353729&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

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

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