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

Inchi: InChI=1S/C16H22F8O4/c1-4-7-8-27-11(25)13(5-2,6-3)12(26)28-9-14(19,20)16(23,24)15(

InchiKey: ZGMPOSGSTMVCIL-UHFFFAOYSA-N

Formula: C16H22F8O4

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

Mol. weight [g/mol]: 430.33

Physical Properties

Property code	Value	Unit	Source
gf	-1933.56	kJ/mol	Joback Method
hf	-2472.33	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.850		Crippen Method
mcvol	265.340	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
tb	698.86	K	Joback Method
tc	863.27	K	Joback Method
tf	413.80	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.28	J/mol×K	698.86	Joback Method
cpg	819.56	J/mol×K	726.26	Joback Method
cpg	832.99	J/mol×K	753.66	Joback Method
cpg	845.60	J/mol×K	781.07	Joback Method
cpg	857.44	J/mol×K	808.47	Joback Method
cpg	868.57	J/mol×K	835.87	Joback Method
cpg	879.02	J/mol×K	863.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370652&Units=SI

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