Malonic acid, decyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C18H26F8O4/c1-2-3-4-5-6-7-8-9-10-29-13(27)11-14(28)30-12-16(21,22)18(25

InchiKey: DDGPXWDETMCOGA-UHFFFAOYSA-N

Formula: C18H26F8O4

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

Mol. weight [g/mol]: 458.38

Physical Properties

Property code	Value	Unit	Source
gf	-1919.56	kJ/mol	Joback Method
hf	-2504.86	kJ/mol	Joback Method
hfus	46.82	kJ/mol	Joback Method
hvap	63.16	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.775		Crippen Method
mcvol	293.520	ml/mol	McGowan Method
pc	1008.45	kPa	Joback Method
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook
tb	747.85	K	Joback Method
tc	916.31	K	Joback Method
tf	433.92	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.96	J/mol×K	747.85	Joback Method
cpg	931.19	J/mol×K	775.93	Joback Method
cpg	945.53	J/mol×K	804.00	Joback Method
cpg	959.02	J/mol×K	832.08	Joback Method
cpg	971.71	J/mol×K	860.16	Joback Method
cpg	983.64	J/mol×K	888.24	Joback Method
cpg	994.86	J/mol×K	916.31	Joback Method

Sources

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=U349354&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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