Diethylmalonic acid, octyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C18H30F4O4/c1-4-7-8-9-10-11-12-25-15(23)17(5-2,6-3)16(24)26-13-18(21,22)14(19)20/h14H,4-13H2,1-3H3

InchiKey: PMRYSILXJASHAC-UHFFFAOYSA-N

Formula: C18H30F4O4

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

Mol. weight [g/mol]: 386.42

Physical Properties

Property code	Value	Unit	Source
gf	-1143.16	kJ/mol	Joback Method
hf	-1711.67	kJ/mol	Joback Method
hfus	41.92	kJ/mol	Joback Method
hvap	67.73	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.140		Crippen Method
mcvol	286.440	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	1751.00		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	754.00	K	Joback Method
tc	928.27	K	Joback Method
tf	429.14	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.62	J/mol×K	754.00	Joback Method
cpg	899.87	J/mol×K	783.05	Joback Method
cpg	915.21	J/mol×K	812.09	Joback Method
cpg	929.67	J/mol×K	841.14	Joback Method
cpg	943.29	J/mol×K	870.18	Joback Method
cpg	956.09	J/mol×K	899.23	Joback Method
cpg	968.13	J/mol×K	928.27	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=U370836&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