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

Inchi: InChI=1S/C17H28F4O4/c1-4-7-8-9-10-11-24-14(22)16(5-2,6-3)15(23)25-12-17(20,21)13

InchiKey: BYCXYUBUZILGKB-UHFFFAOYSA-N

Formula: C17H28F4O4

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

Mol. weight [g/mol]: 372.40

Physical Properties

Property code	Value	Unit	Source
gf	-1151.58	kJ/mol	Joback Method
hf	-1691.03	kJ/mol	Joback Method
hfus	39.33	kJ/mol	Joback Method
hvap	65.50	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.750		Crippen Method
mcvol	272.350	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
tb	731.12	K	Joback Method
tc	903.33	K	Joback Method
tf	417.87	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.03	J/mol×K	731.12	Joback Method
cpg	841.86	J/mol×K	759.82	Joback Method
cpg	856.82	J/mol×K	788.52	Joback Method
cpg	870.94	J/mol×K	817.23	Joback Method
cpg	884.24	J/mol×K	845.93	Joback Method
cpg	896.77	J/mol×K	874.63	Joback Method
cpg	908.55	J/mol×K	903.33	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=U370835&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