Diethylmalonic acid, 2,2,3,3,4,4,4-heptafluorobutyl tetradecyl ester

Inchi: InChI=1S/C25H41F7O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-35-20(33)22(5-2,6-3)21

InchiKey: FXJKTIMAWRGRBA-UHFFFAOYSA-N

Formula: C25H41F7O4

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

Mol. weight [g/mol]: 538.58

Physical Properties

Property code	Value	Unit	Source
gf	-1660.53	kJ/mol	Joback Method
hf	-2456.70	kJ/mol	Joback Method
hfus	57.98	kJ/mol	Joback Method
hvap	78.65	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	8.413		Crippen Method
mcvol	390.380	ml/mol	McGowan Method
pc	705.46	kPa	Joback Method
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
tb	905.95	K	Joback Method
tc	1117.10	K	Joback Method
tf	529.64	K	Joback Method
vc	1.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1330.13	J/mol×K	905.95	Joback Method
cpg	1349.64	J/mol×K	941.14	Joback Method
cpg	1367.88	J/mol×K	976.33	Joback Method
cpg	1384.99	J/mol×K	1011.52	Joback Method
cpg	1401.10	J/mol×K	1046.72	Joback Method
cpg	1416.33	J/mol×K	1081.91	Joback Method
cpg	1430.81	J/mol×K	1117.10	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=U368439&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