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

Inchi: InChI=1S/C14H22F4O4/c1-5-13(6-2,11(19)21-7-9(3)4)12(20)22-8-14(17,18)10(15)16/h9-

InchiKey: DADYJHRGEFTVJH-UHFFFAOYSA-N

Formula: C14H22F4O4

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

Mol. weight [g/mol]: 330.32

Physical Properties

Property code	Value	Unit	Source
gf	-1179.28	kJ/mol	Joback Method
hf	-1634.39	kJ/mol	Joback Method
hfus	28.04	kJ/mol	Joback Method
hvap	58.43	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.436		Crippen Method
mcvol	230.080	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook
tb	662.04	K	Joback Method
tc	833.58	K	Joback Method
tf	369.06	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.03	J/mol×K	662.04	Joback Method
cpg	674.83	J/mol×K	690.63	Joback Method
cpg	688.82	J/mol×K	719.22	Joback Method
cpg	702.03	J/mol×K	747.81	Joback Method
cpg	714.48	J/mol×K	776.40	Joback Method
cpg	726.21	J/mol×K	804.99	Joback Method
cpg	737.24	J/mol×K	833.58	Joback Method

Sources

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=U370831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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