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

Inchi: InChI=1S/C21H33F7O4/c1-4-7-8-9-10-11-12-13-14-31-16(29)18(5-2,6-3)17(30)32-15-19

InchiKey: DQCYAWQCXJMHAF-UHFFFAOYSA-N

Formula: C21H33F7O4

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

Mol. weight [g/mol]: 482.47

Physical Properties

Property code	Value	Unit	Source
gf	-1694.21	kJ/mol	Joback Method
hf	-2374.14	kJ/mol	Joback Method
hfus	47.62	kJ/mol	Joback Method
hvap	69.75	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.853		Crippen Method
mcvol	334.020	ml/mol	McGowan Method
pc	874.80	kPa	Joback Method
rinpol	1904.00		NIST Webbook
rinpol	1904.00		NIST Webbook
tb	814.43	K	Joback Method
tc	997.09	K	Joback Method
tf	484.56	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.38	J/mol×K	814.43	Joback Method
cpg	1102.13	J/mol×K	844.87	Joback Method
cpg	1117.85	J/mol×K	875.32	Joback Method
cpg	1132.62	J/mol×K	905.76	Joback Method
cpg	1146.52	J/mol×K	936.20	Joback Method
cpg	1159.62	J/mol×K	966.65	Joback Method
cpg	1172.00	J/mol×K	997.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368435&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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