

Diethylmalonic acid, 2,2,3,3,4,4,5,5-octafluoropentyl hexadecyl

Inchi:
ester

InChI=1S/C28H46F8O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-39-23(37)25(5-2,

InchiKey:

FTWCBGRWQBGSRC-UHFFFAOYSA-N

Formula:

C28H46F8O4

SMILES:

CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]:

598.65

Physical Properties

Property code	Value	Unit	Source
gf	-1832.52	kJ/mol	Joback Method
hf	-2720.01	kJ/mol	Joback Method
hfus	65.31	kJ/mol	Joback Method
hvap	84.13	kJ/mol	Joback Method
log10ws	-10.28		Crippen Method
logp	9.532		Crippen Method
mvol	434.420	ml/mol	McGowan Method
pc	597.80	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	973.42	K	Joback Method
tc	1221.73	K	Joback Method
tf	549.04	K	Joback Method
vc	1.746	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1527.17	J/mol×K	973.42	Joback Method
cpg	1549.78	J/mol×K	1014.80	Joback Method
cpg	1570.82	J/mol×K	1056.19	Joback Method
cpg	1590.51	J/mol×K	1097.57	Joback Method
cpg	1609.07	J/mol×K	1138.96	Joback Method
cpg	1626.73	J/mol×K	1180.34	Joback Method
cpg	1643.71	J/mol×K	1221.73	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=U370664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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