

Diethylmalonic acid, dodecyl 2,4,5-trifluorobenzyl ester

Inchi:	InChI=1S/C26H39F3O4/c1-4-7-8-9-10-11-12-13-14-15-16-32-24(30)26(5-2,6-3)25(31)33
InchiKey:	XEDXKUQVDVZTDW-UHFFFAOYSA-N
Formula:	C26H39F3O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cc(F)c(F)cc1F
Mol. weight [g/mol]:	472.58

Physical Properties

Property code	Value	Unit	Source
gf	-797.87	kJ/mol	Joback Method
hf	-1464.53	kJ/mol	Joback Method
hfus	63.37	kJ/mol	Joback Method
hvap	92.30	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	7.418		Crippen Method
mvol	373.630	ml/mol	McGowan Method
pc	839.19	kPa	Joback Method
rinpol	2674.00		NIST Webbook
tb	983.06	K	Joback Method
tc	1206.89	K	Joback Method
tf	595.27	K	Joback Method
vc	1.474	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1262.80	J/molxK	983.06	Joback Method
cpg	1279.92	J/molxK	1020.36	Joback Method
cpg	1295.54	J/molxK	1057.67	Joback Method
cpg	1309.72	J/molxK	1094.97	Joback Method
cpg	1322.54	J/molxK	1132.28	Joback Method
cpg	1334.04	J/molxK	1169.58	Joback Method
cpg	1344.31	J/molxK	1206.89	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=U369263&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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