

# Diethylmalonic acid, 1-bromo-3,3,3-trifluoroprop-2-yl pentyl ester

Inchi:	InChI=1S/C15H24BrF3O4/c1-4-7-8-9-22-12(20)14(5-2,6-3)13(21)23-11(10-16)15(17,18)
InchiKey:	LVZDUPSSGBEDE-UHFFFAOYSA-N
Formula:	C15H24BrF3O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OC(CBr)C(F)(F)F
Mol. weight [g/mol]:	405.25

## Physical Properties

Property code	Value	Unit	Source
gf	-959.29	kJ/mol	Joback Method
hf	-1427.31	kJ/mol	Joback Method
hfus	36.35	kJ/mol	Joback Method
hvap	68.30	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.395		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpola	1659.00		NIST Webbook
rinpola	1659.00		NIST Webbook
tb	752.25	K	Joback Method
tc	938.03	K	Joback Method
tf	454.54	K	Joback Method
vc	1.012	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.07	J/molxK	752.25	Joback Method
cpg	765.16	J/molxK	783.21	Joback Method
cpg	778.40	J/molxK	814.18	Joback Method
cpg	790.81	J/molxK	845.14	Joback Method
cpg	802.44	J/molxK	876.10	Joback Method
cpg	813.33	J/molxK	907.07	Joback Method
cpg	823.52	J/molxK	938.03	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U370796&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370796&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rlnol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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