

1-Ethyl-2-heptafluorobutyryloxycyclohexane

Inchi:	InChI=1S/C12H15F7O2/c1-2-7-5-3-4-6-8(7)21-9(20)10(13,14)11(15,16)12(17,18)19/h7-8
InchiKey:	QUGSZKGFYRCIMJ-UHFFFAOYSA-N
Formula:	C12H15F7O2
SMILES:	CCC1CCCCC1OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	324.24

Physical Properties

Property code	Value	Unit	Source
hfus	21.85	kJ/mol	Joback Method
logp	4.331		Crippen Method
mcvol	188.910	ml/mol	McGowan Method
rinpol	1079.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.28	J/mol×K	550.33	Joback Method
cpg	537.25	J/mol×K	578.86	Joback Method
cpg	553.20	J/mol×K	607.39	Joback Method
cpg	568.17	J/mol×K	635.92	Joback Method
cpg	582.20	J/mol×K	664.45	Joback Method
cpg	595.34	J/mol×K	692.98	Joback Method
cpg	607.62	J/mol×K	721.51	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C959079926&Units=SI>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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