

2-(2-Ethoxyethoxy)ethyl 2,2,3,3,4,4,4-heptafluorobutanoate

Other names: Diethylene glycol monoethyl ether, heptafluorobutyrate

3,6-Dioxaoct-1-yl heptafluorobutyrate

Inchi: InChI=1S/C10H13F7O4/c1-2-19-3-4-20-5-6-21-7(18)8(11,12)9(13,14)10(15,16)17/h2-6H

InchiKey: XMZPTRSHHDNMHU-UHFFFAOYSA-N

Formula: C10H13F7O4

SMILES: CCOCCOCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 330.20

Physical Properties

Property code	Value	Unit	Source
gf	-1765.75	kJ/mol	Joback Method
hf	-2157.99	kJ/mol	Joback Method
hfus	26.14	kJ/mol	Joback Method
hvap	42.22	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.416		Crippen Method
mcvol	183.330	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	1088.60		NIST Webbook
rinpol	1088.60		NIST Webbook
tb	534.53	K	Joback Method
tc	683.91	K	Joback Method
tf	330.47	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.99	J/molxK	534.53	Joback Method
cpg	499.25	J/molxK	559.43	Joback Method
cpg	510.91	J/molxK	584.32	Joback Method
cpg	521.99	J/molxK	609.22	Joback Method
cpg	532.52	J/molxK	634.12	Joback Method
cpg	542.49	J/molxK	659.02	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=U352016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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