

heptafluorobutanoic acid, heptadecyl ester

Other names:	Heptadecyl 2,2,3,3,4,4,4-heptafluorobutanoate 1-Heptadecanol, heptafluorobutyrate Heptadecyl perfluorobutyrate Heptafluorobutyric acid, heptadecyl ester
Inchi:	InChI=1S/C21H35F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-30-18(29)19(22,23)
InchiKey:	JMANSDFHCFBZBM-UHFFFAOYSA-N
Formula:	C21H35F7O2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	452.49

Physical Properties

Property code	Value	Unit	Source
hf	-2183.13	kJ/mol	Cheméo Relay (1.0)
hfus	52.25	kJ/mol	Joback Method
hvap	99.32	kJ/mol	Cheméo Relay (1.0)
log10ws	-8.31		Cheméo Relay (1.0)
logp	8.234		Crippen Method
mcvol	326.580	ml/mol	McGowan Method
pc	842.11	kPa	Joback Method
rinpol	1938.00		NIST Webbook
rinpol	1941.40		NIST Webbook
rinpol	1938.00		NIST Webbook
tb	568.11	K	Cheméo Relay (1.0)
tc	677.95	K	Cheméo Relay (1.0)
tf	273.60	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.37	J/mol×K	741.37	Joback Method
cpg	1044.61	J/mol×K	769.12	Joback Method
cpg	1061.89	J/mol×K	796.86	Joback Method
cpg	1078.25	J/mol×K	824.61	Joback Method
cpg	1093.76	J/mol×K	852.35	Joback Method

cpg	1108.47	J/mol×K	880.10	Joback Method
cpg	1122.43	J/mol×K	907.84	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C959085666&Units=SI>

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/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
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

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