2-Heptynyl aldehyde diethyl acetal

Inchi: InChI=1S/C11H20O2/c1-4-7-8-9-10-11(12-5-2)13-6-3/h11H,4-8H2,1-3H3
InchiKey: NKXTVBJJMIROGV-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: CCCCC#CC(OCC)OCC
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
hf	-248.53	kJ/mol	Cheméo Relay (1.0)
hfus	26.22	kJ/mol	Joback Method
hvap	59.10	kJ/mol	Cheméo Relay (1.0)
ie	9.33	eV	Cheméo Relay (1.0)
logp	2.579		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
tb	456.75	K	Cheméo Relay (1.0)
tf	200.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.97	J/mol×K	504.48	Joback Method
cpg	399.23	J/mol×K	535.31	Joback Method
cpg	413.96	J/mol×K	566.14	Joback Method
cpg	428.15	J/mol×K	596.96	Joback Method
cpg	441.80	J/mol×K	627.79	Joback Method
cpg	454.91	J/mol×K	658.62	Joback Method
cpg	467.47	J/mol×K	689.45	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18232309&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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