

2-(2-Butoxyethoxy)ethyl 3,5,5-trimethylhexanoate

Inchi:	InChI=1S/C17H34O4/c1-6-7-8-19-9-10-20-11-12-21-16(18)13-15(2)14-17(3,4)5/h15H,6-
InchiKey:	HXJMQMMAHSUMPT-UHFFFAOYSA-N
Formula:	C17H34O4
SMILES:	CCCCOCCOCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	302.45

Physical Properties

Property code	Value	Unit	Source
gf	-351.26	kJ/mol	Joback Method
hf	-917.48	kJ/mol	Joback Method
hfus	34.01	kJ/mol	Joback Method
hvap	65.73	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.825		Crippen Method
mvol	269.570	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	1875.00		NIST Webbook
tb	705.82	K	Joback Method
tc	882.49	K	Joback Method
tf	385.39	K	Joback Method
vc	1.030	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.64	J/molxK	705.82	Joback Method
cpg	816.13	J/molxK	735.27	Joback Method
cpg	833.71	J/molxK	764.71	Joback Method
cpg	850.38	J/molxK	794.16	Joback Method
cpg	866.17	J/molxK	823.60	Joback Method
cpg	881.08	J/molxK	853.05	Joback Method
cpg	895.13	J/molxK	882.49	Joback Method
dvisc	0.0013340	Paxs	385.39	Joback Method
dvisc	0.0005506	Paxs	438.79	Joback Method

dvisc	0.0002754	Paxs	492.20	Joback Method
dvisc	0.0001577	Paxs	545.61	Joback Method
dvisc	0.0000998	Paxs	599.01	Joback Method
dvisc	0.0000680	Paxs	652.41	Joback Method
dvisc	0.0000492	Paxs	705.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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